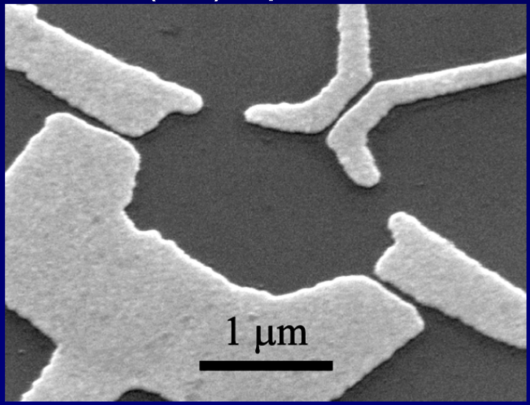
Lecture 18:
3D Review, Examples

A real (2D) "quantum dot"



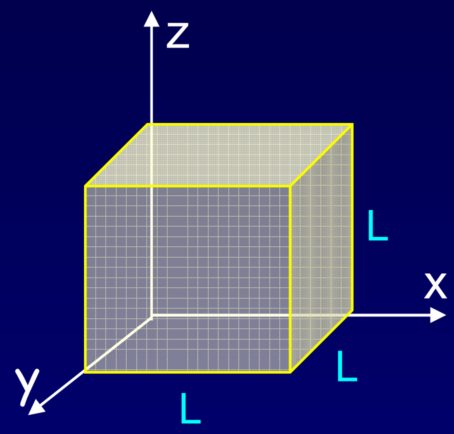
http://pages.unibas.ch/phys-meso/Pictures/pictures.html

Lect. 16: Particle in a 3D Box (3)

The energy eigenstates and energy values in a 3D cubical box are:

$$\boxed{\begin{aligned}\psi &= N \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) \sin\left(\frac{n_z \pi}{L} z\right) \\ E_{n_x n_y n_z} &= \frac{h^2}{8mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)\end{aligned}}$$

where n_x, n_y, and n_z can each have values 1,2,3,….



This problem illustrates two important points:

- **Three quantum numbers (n_x,n_y,n_z) are needed to identify the state of this three-dimensional system.**
  That is true for every 3D system.

- **More than one state can have the same energy: "Degeneracy".**
  Degeneracy reflects an underlying symmetry in the problem.
  3 equivalent directions, because it's a cube, not a rectangle.

Act 1

Consider a particle in a 2D well, with $L_x = L_y = L$.

1. Compare the energies of the (2,2), (1,3), and (3,1) states?
   a. $E_{(2,2)} > E_{(1,3)} = E_{(3,1)}$
   b. $E_{(2,2)} = E_{(1,3)} = E_{(3,1)}$
   c. $E_{(2,2)} < E_{(1,3)} = E_{(3,1)}$

2. If we squeeze the box in the x-direction (*i.e.*, $L_x < L_y$) compare $E_{(1,3)}$ with $E_{(3,1)}$.
   a. $E_{(1,3)} < E_{(3,1)}$
   b. $E_{(1,3)} = E_{(3,1)}$
   c. $E_{(1,3)} > E_{(3,1)}$

Solution

Consider a particle in a 2D well, with $L_x = L_y = L$.

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   c. $\boxed{E_{(2,2)} < E_{(1,3)} = E_{(3,1)}}$

$$E_{(1,3)} = E_{(3,1)} = E_0\,(1^2 + 3^2) = 10\,E_0$$

$$E_{(2,2)} = E_0\,(2^2 + 2^2) = 8\,E_0$$

$$E_0 \equiv \frac{h^2}{8mL^2}$$

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   a. $\boxed{E_{(1,3)} < E_{(3,1)}}$
   b. $E_{(1,3)} = E_{(3,1)}$
   c. $E_{(1,3)} > E_{(3,1)}$

Because $L_x < L_y$, for a given n, E_0 for x motion is larger than E_0 for y motion. The effect is larger for larger n. Therefore, $E_{(3,1)} > E_{(1,3)}$.

Example: $L_x = ½$, $L_y = 1$:

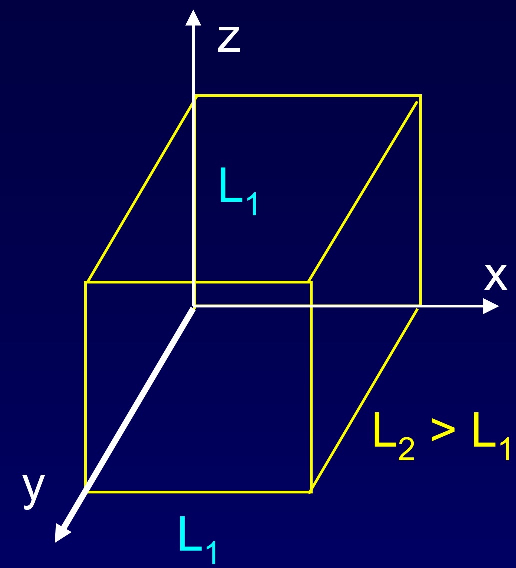
$E_{(1,3)} \propto 4\times1^2 + 1\times3^2 = 13$
$E_{(3,1)} \propto 4\times3^2 + 1\times1^2 = 37$

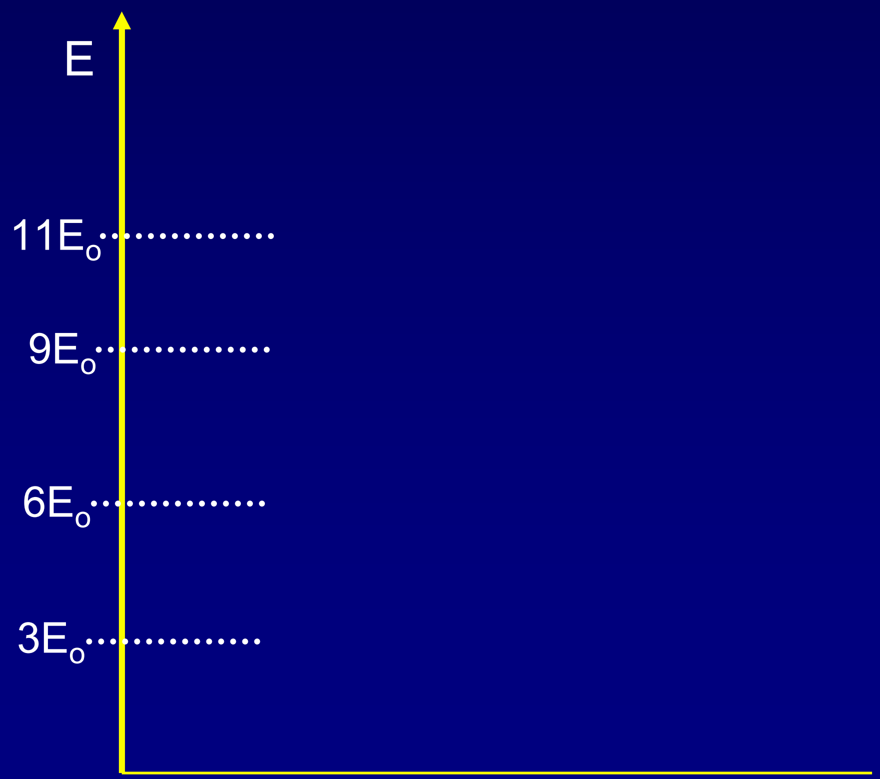
We say "the degeneracy has been lifted."

Non-cubic Box

Consider a non-cubic box:

The box is stretched along the y-direction.
What will happen to the energy levels?
Define $E_o = h^2/8mL_1^2$





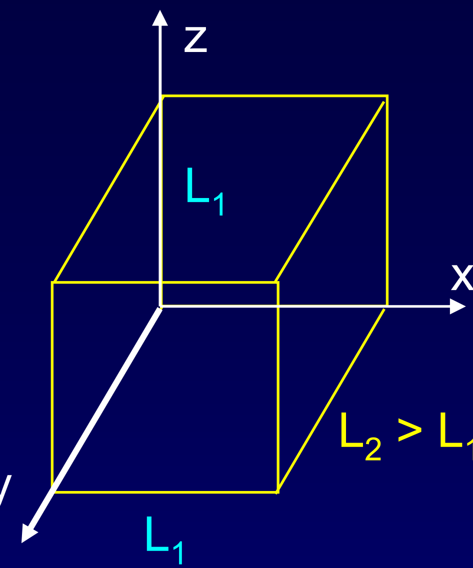
Solution

Consider a non-cubic box:

The box is stretched along the y-direction.

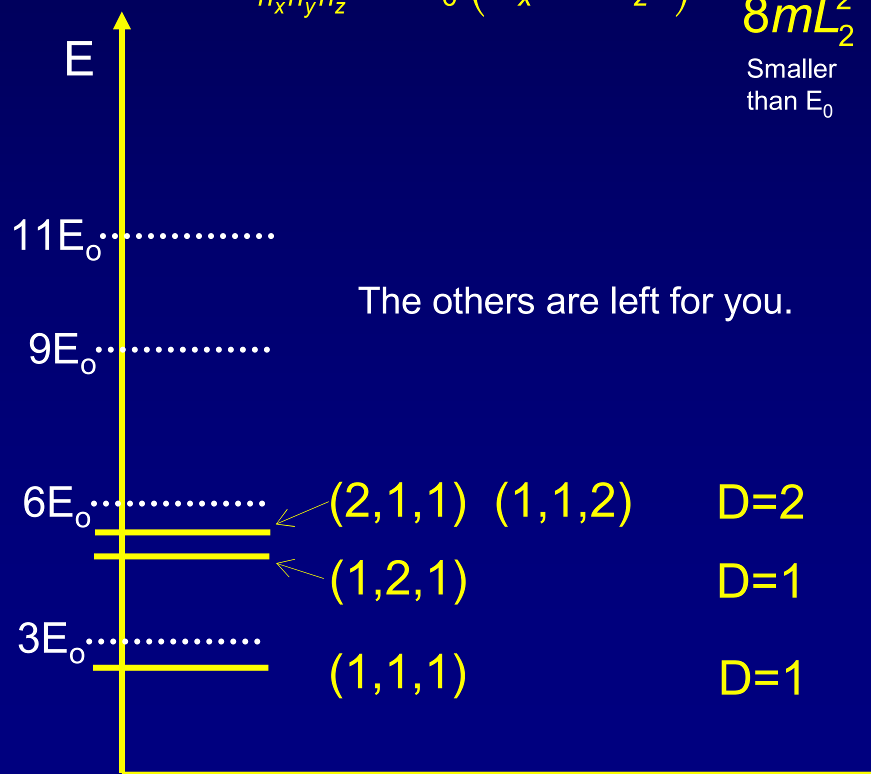
What will happen to the energy levels?

Define $E_o = h^2/8mL_1^2$



$$E_{n_x n_y n_z} = E_0\left(n_x^{\ 2} + n_z^{\ 2}\right) + \frac{h^2}{8mL_2^2}\left(n_y^{\ 2}\right)$$

Smaller than E_0



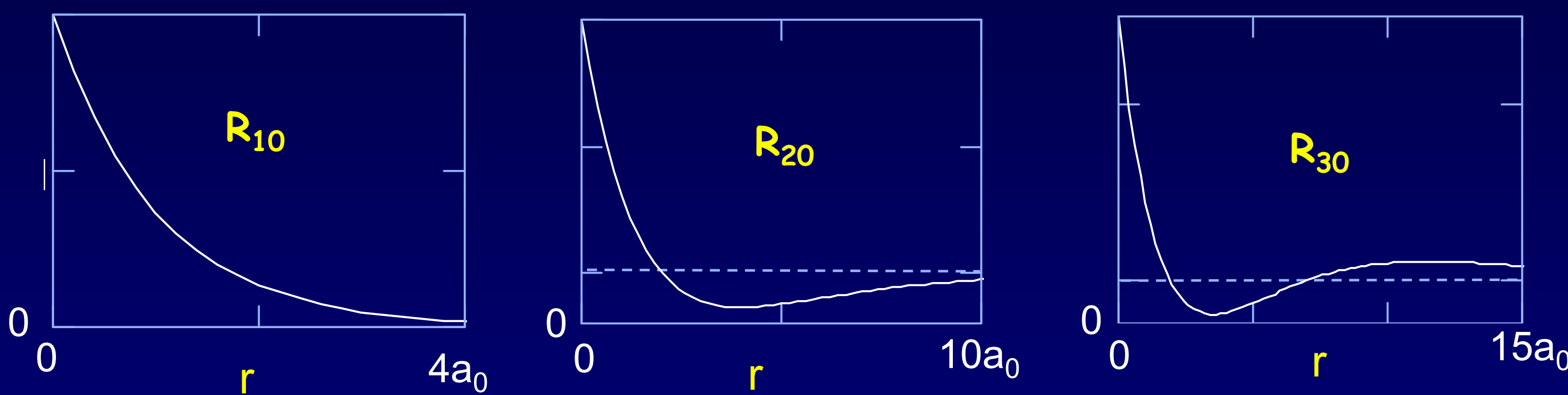
The others are left for you.

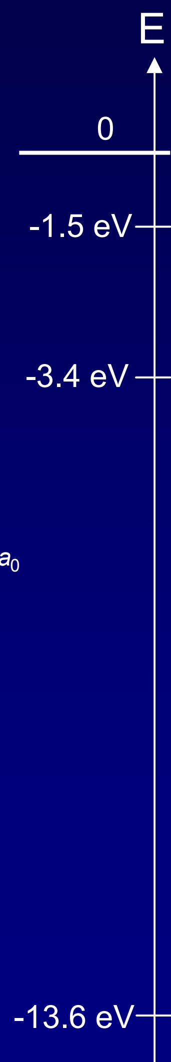
1: The symmetry is "broken" for y, so the 3-fold degeneracy is lowered. A 2-fold degeneracy remains, because x and z are still symmetric.

2: There is an overall lowering of energies due to decreased confinement along y.

Radial Eigenstates of Hydrogen

Here are graphs of the s-state wave functions, $R_{no}(r)$, for the electron in the Coulomb potential of the proton. The zeros in the subscripts are a reminder that these are states with $l = 0$ (zero angular momentum!).





$$R_{1,0}(r) \propto e^{-r/a_0}$$

$$R_{2,0}(r) \propto \left(1 - \frac{r}{2a_0}\right) e^{-r/2a_0}$$

$$R_{3,0}(r) \propto \left(3 - \frac{2r}{a_0} + 2\left(\frac{r}{3a_0}\right)^2\right) e^{-r/3a_0}$$

$$\boxed{r \approx \frac{\hbar^2}{m\kappa e^2} \equiv a_0 = 0.053\text{ nm}}$$

The "Bohr radius" of the H atom.

$$\boxed{E \approx -\frac{m\kappa^2 e^4}{2\hbar^2} = -13.6\text{ eV}}$$

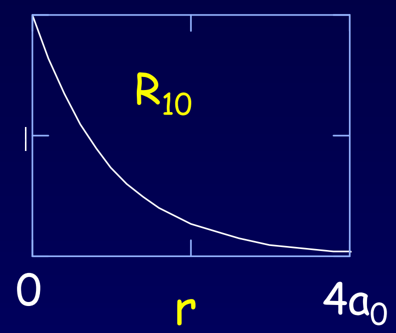
The ground state energy of the hydrogen atom.

One factor of e or e^2 comes from the proton charge, and one from the electron.

Wave Function Normalization

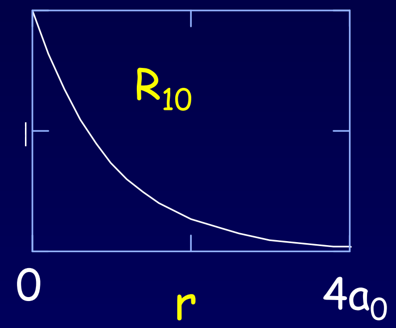
What is the normalization constant for the hydrogen atom ground state?

$$\psi_{100}(r,\theta,\phi) = NR_{10}(r) = Ne^{-r/a_o}$$



Solution

What is the normalization constant for the hydrogen atom ground state?



$$\psi_{100}(r,\theta,\phi) = NR_{10}(r) = Ne^{-r/a_o}$$

The probability density is $|\psi|^2 = N^2 \exp(-2r/a_o)$.
In 3D, this means "probability per unit volume".

We require that the total probability = 1: $\int |\psi|^2 \, dV = 1$

$dV = r^2 \sin\theta \, dr \, d\theta \, d\phi$

With spherical symmetry, the angular integrals give 4π, so we are left with:

$$4\pi N^2 \int_0^\infty r^2 e^{-2r/a_0} dr = 1 \quad \Rightarrow \quad N^2 = \frac{1}{\pi a_o^3}$$

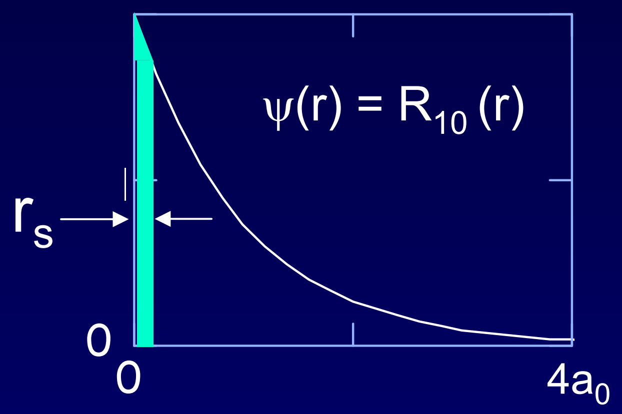
"You can look it up!"

$$\boxed{\psi_{100}(r) = \sqrt{\frac{1}{\pi a_o^3}} \; e^{-r/a_o}}$$

Normalized ground-state wave function of hydrogen

Probability Calculation

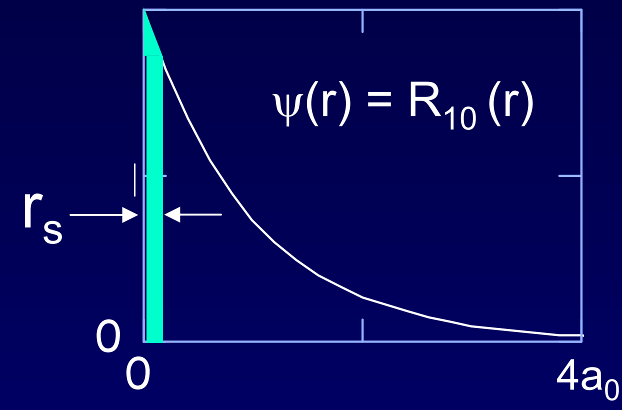
Estimate the probability of finding the electron within a small sphere of radius r_s = 0.2 a_o at the origin.



$$\psi(r) = Ne^{-r/a_o}$$

Solution

Estimate the probability of finding the electron within a small sphere of radius $r_s = 0.2\ a_o$ at the origin.



If it says "estimate", don't integrate.

The wave function is nearly constant near r = 0:

$$\psi(0) = \sqrt{\frac{1}{\pi a_o^3}}\, e^{-0/a_o} = \sqrt{\frac{1}{\pi a_o^3}}$$

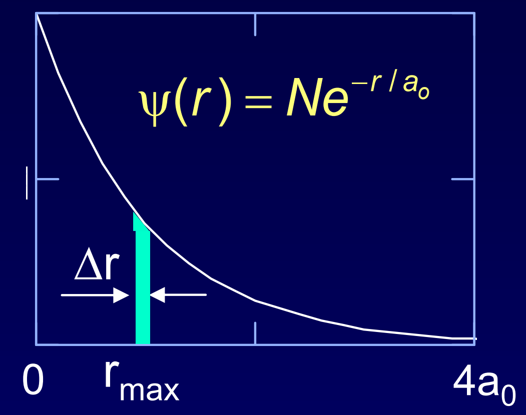
$$\psi(r) = Ne^{-r/a_o}$$

Simply multiply $|\psi|^2$ by the volume $\Delta V = (4/3)\pi r_s^3$:

$$\text{Probability} = |\psi(0)|^2 \Delta V = \frac{4}{3}\left(\frac{r_s}{a_o}\right)^3 \approx 0.01$$

Maximum Radial Probability

At what radius are you most likely to find the electron?



Solution

At what radius are you most likely to find the electron?

Looks like a no-brainer. $r = 0$, of course!

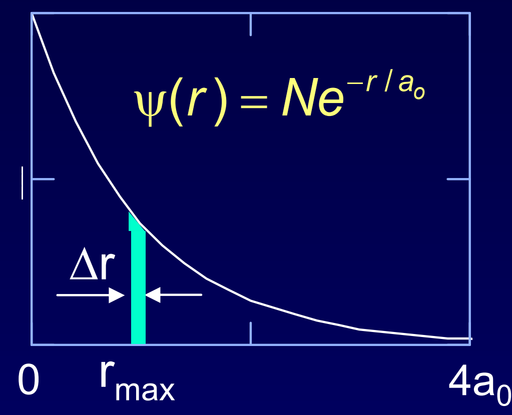
Well, that's not the answer.

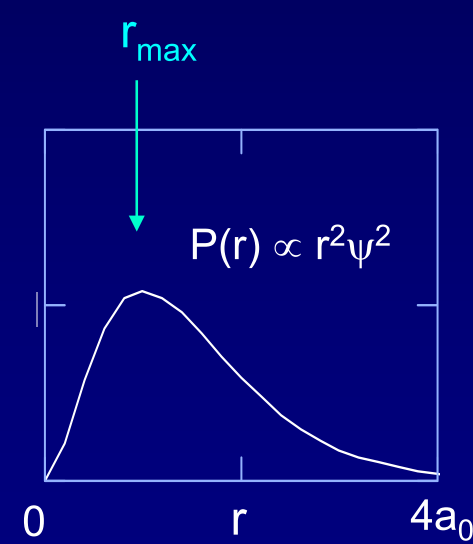
You must find the probability $P(r)\Delta r$ that the electron is in a shell of thickness Δr at radius r. For a given Δr the volume, ΔV, of the shell increases with radius.

The radial probability has an extra factor of r^2:

$$P(r)\Delta r = |\psi(r)|^2\,\Delta V = Cr^2 e^{-2r/a_o}\,\Delta r$$

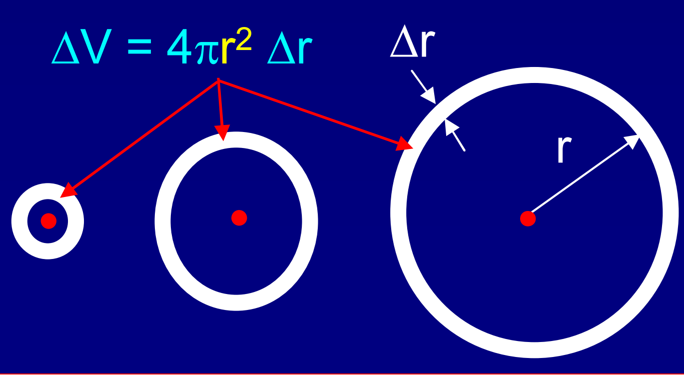
Set $dP/dr = 0$ to find: $\boxed{r_{max} = a_0\ !}$





More volume at larger r.

No volume at r = 0.



Act 2

Consider an electron around a nucleus that has two protons, like an ionized Helium atom.

1. Compare the "effective Bohr radius" $a_{0,He}$ with the usual Bohr radius for hydrogen, a_0:
   a. $a_{0,He} > a_0$
   b. $a_{0,He} = a_0$
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$$r \approx \frac{\hbar^2}{m\kappa e^2} \equiv a_0 = 0.053 \text{ nm}$$

The "Bohr radius" of the H atom.

2. What is the ratio of ground state energies $E_{0,He}/E_{0,H}$?
   a. $E_{0,He}/E_{0,H} = 1$
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   c. $\boxed{a_{0,He} < a_0}$

Look at how a_0 depends on the charge:

$$a_0 \equiv \frac{\hbar^2}{m\kappa e^2} \Rightarrow a_{0,He} \equiv \frac{\hbar^2}{m\kappa(2e)e} = \frac{a_0}{2}$$

This should make sense:
more charge → stronger attraction
→ electron sits closer to the nucleus

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   c. $\boxed{E_{0,He}/E_{0,H} = 4}$

Clearly the electron will be more tightly bound, so $|E_{0,He}| > |E_{0,H}|$. How much more tightly? Look at E_0:

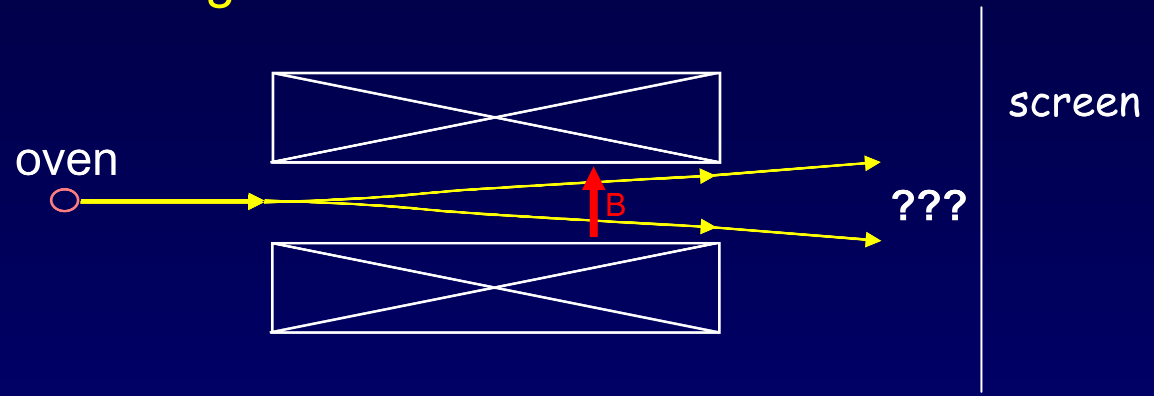
$$E_{0,H} = -\frac{m\kappa^2 e^4}{2\hbar^2} \quad \Rightarrow \quad E_{0,He} = \frac{-m\kappa^2 (2e)^2 e^2}{2\hbar^2} = 4E_{0,H}$$

In general, for a "hydrogenic" atom (only one electron) with Z protons:

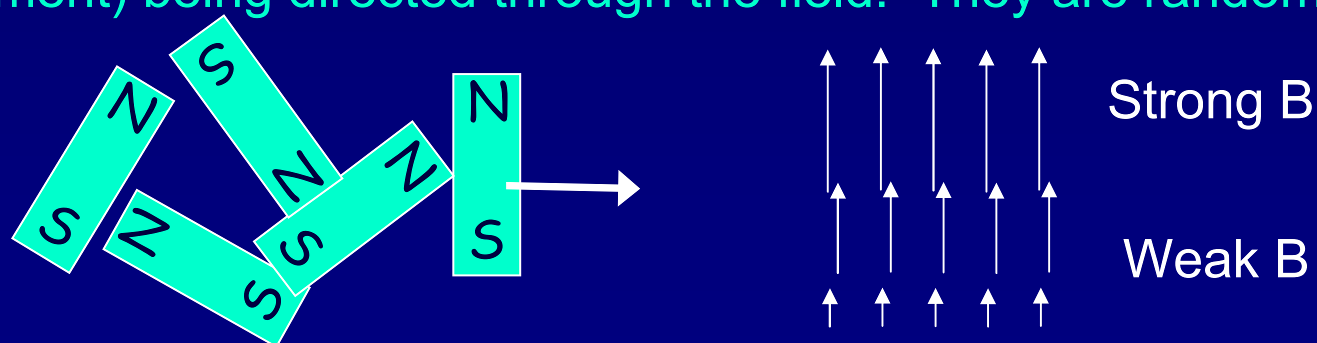
$$\boxed{E_{0,Z} = Z^2 E_{0,H}}$$

Stern-Gerlach Experiment & Electron Spin

In 1922, Stern and Gerlach shot a beam of Ag atoms (with $l = 0$) through a non-uniform magnetic field and detected them at a screen.

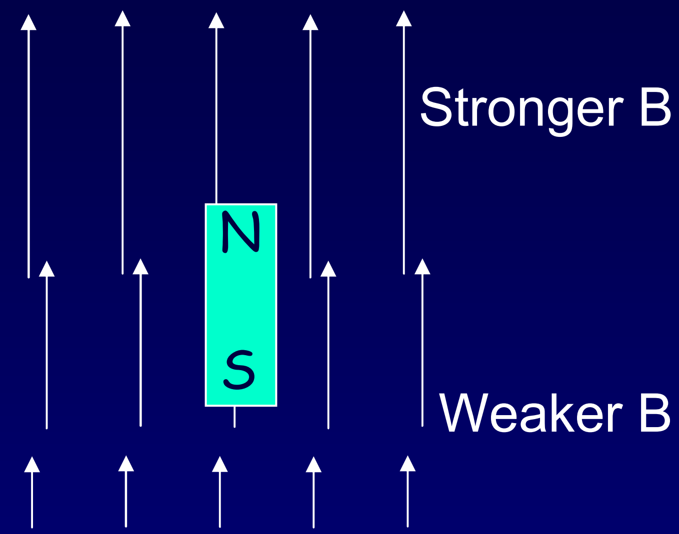


We can think of the atoms as tiny magnets (they have a magnetic moment) being directed through the field. They are randomly oriented:



Act 3

1. Consider a magnet in an inhomogeneous field, as shown.
   Which way will the magnet feel a force?



a. Up
b. Down
c. Left
d. Right
e. No force

2. The magnets (i.e., atoms) leave the oven with random orientations.
   What pattern do you expect on the screen?

Solution

1. Consider a magnet in an inhomogeneous field, as shown.
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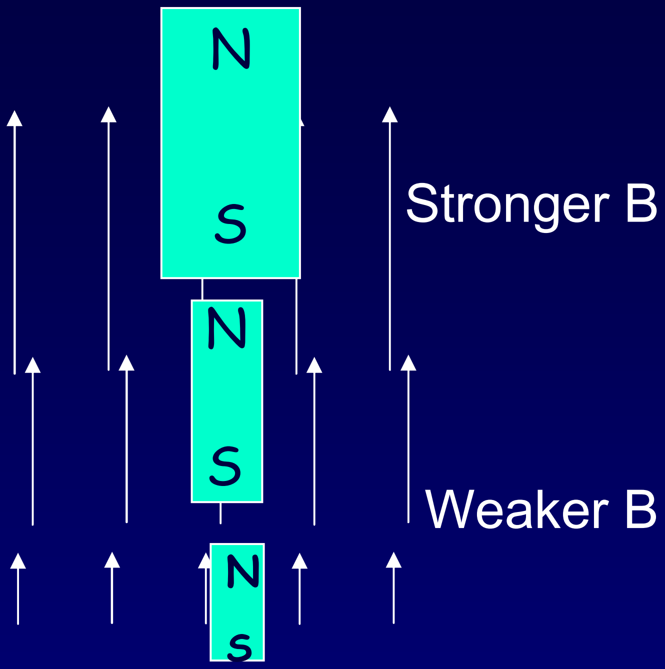

a. $\boxed{\text{Up}}$
b. Down
c. Left
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e. No force

The N pole is in a stronger field than the S pole, so its upward force dominates.

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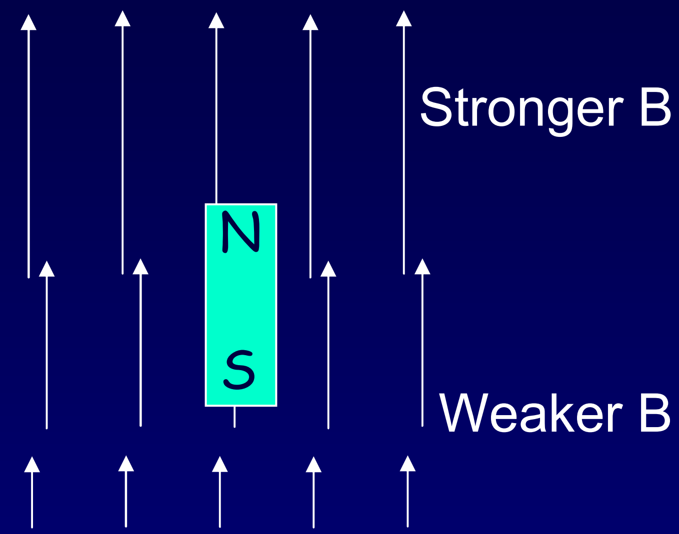

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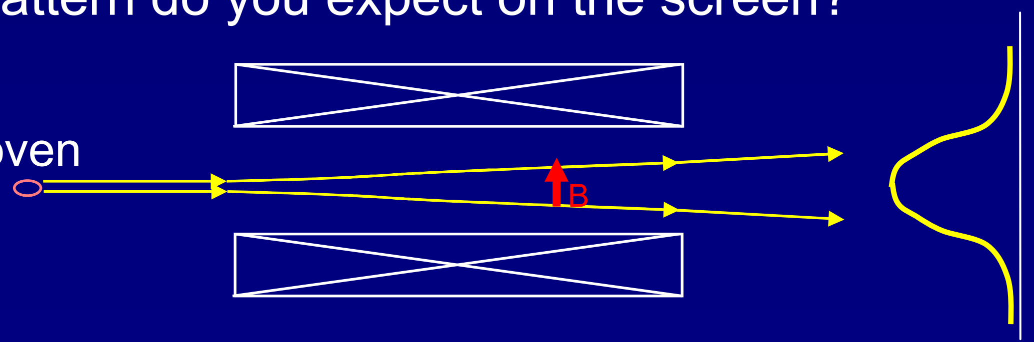
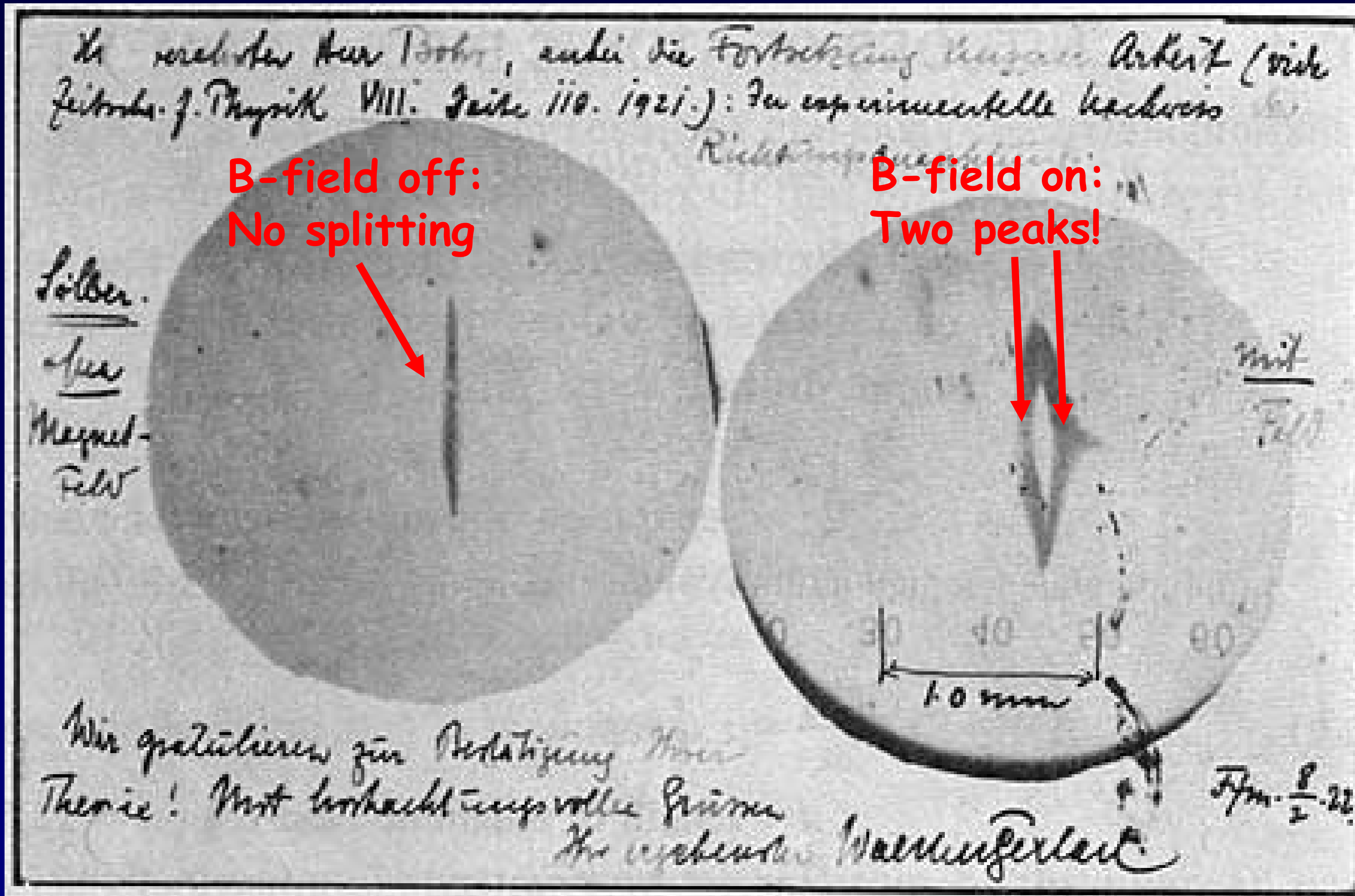
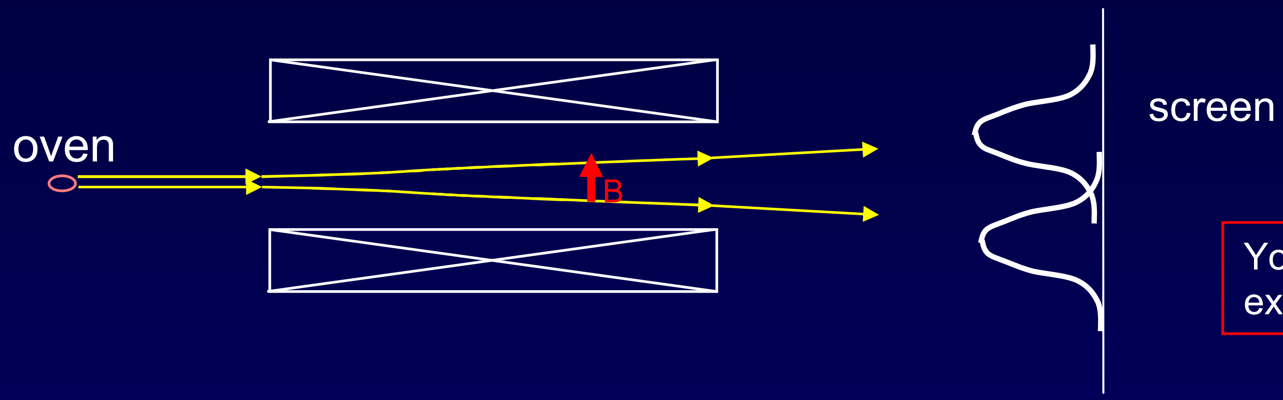


We expect a blob, because the position depends on the random rotation angle.



Gerlach's postcard, dated 8 February 1922, to Niels Bohr. It shows a photograph of the beam splitting, with the message, in translation: “Attached [is] the experimental proof of directional quantization. We congratulate [you] on the confirmation of your theory.”

Back to the Stern-Gerlach Experiment



You will analyze this experiment in discussion.

The beam split in two! This marked the discovery of a new type of angular momentum, with an m_s quantum number that can take on only two values:

$$(s = ½) \quad m_s = \pm ½$$

The new kind of angular momentum is called the electron "SPIN". Why?

If the electron were spinning on its axis, it would have angular momentum and a magnetic moment (because it's charged) regardless of its spatial motion.

However, this "spinning" ball picture is not realistic, because it would require the point-like electron to spin so fast that parts would travel faster than c!

So we can't picture the spin in any simple way … the electron's spin is simply another degree-of-freedom available to electron.

Note: <u>Most</u> particles have spin (protons, neutrons, quarks, photons…)

Electron Spin

We need FOUR quantum numbers to specify the electronic state of a hydrogen atom.

n, l, m_l, m_s (where $m_s = -½$ and $+½$)

Actually, the nucleus (a proton) also has spin, so we must specify its m_s as well …

We'll work some example problems next time.

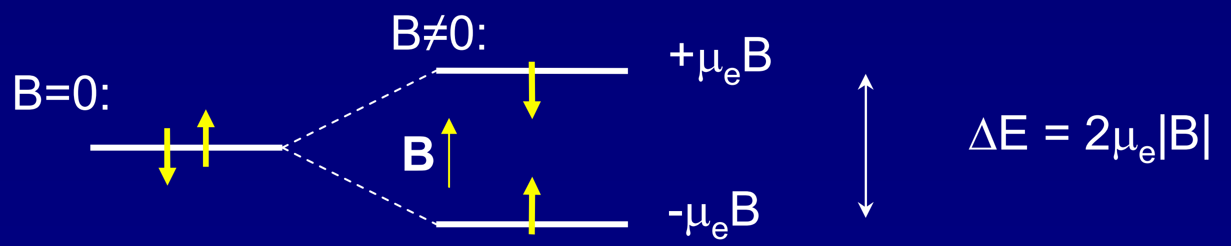
Electron Magnetic Moment

Because the electron has a charge and angular momentum, it has a magnetic moment, with magnitude: $\mu_e = 9.2848\times10^{-24}$ J/T.

One consequence of the 'quantization of angular momentum' is that we only ever measure the spin (and hence the magnetic moment) to be pointing 'up' or 'down' (where the axis is defined by any applied magnetic field). [Note: Because the charge of the electron is negative, the spin and magnetic moment point in *opposite* directions!]

In a uniform magnetic field ($\mathbf{B} = B_z\mathbf{z}$), a magnetic moment has an energy (Phys. 212): $E = -\mu\cdot\mathbf{B} = -\mu_z B_z$

Thus, for an electron, the two spin states have two energies:



Note: These arrows represent magnetic moment, not spin...

FYI: The *real* value of μ_e

- There are relatively simple arguments that predict
  $\mu_e = \mu_B \equiv e\hbar/2m = 9.2740 \times 10^{-24}$ J/T
- In reality, the measured mag. moment of the electron is a bit bigger:
  $\mu_e = -9.2848 \times 10^{-24}$ J/T
- The effect is small:
  $|\mu_e/\mu_B| = 1.00115965218685\ (42)$

[Yes, it has been measured *that* well – in fact, it's one of the most precisely known quantities today.]

- What causes the discrepancy? It comes from the fact that:
  - Magnetic (and electric) effects essentially arise from the exchange of "virtual" photons.
  - Sometimes these can, for a very short time, become an electron-positron pair (which then annihilate each other). There are lots of other exotic processes too.
- When all these are taken into account, our current best theoretical prediction for the value of $|\mu_e/\mu_B| = 1.001159652201\ (27)$
- This is agreement to at least 12 decimal places!!