Quantum Mechanics
Physics 237

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Solving the Schrödinger Equation using Mathematica.

In[1]:= **Solve the finite potential well problem using Mathematica.**

The solution is based on the following text book: Mathematica for Theoretical Physics, Gerd Baumann.

In[1]:=

```
(* Solve the Schroedinger equation in regions 1 and 3 x<-a and x>a. *)
(* The solution is stored in s13. The constant κ is defined as κ = √(2m(V0-E))/ħ *)
s13 = DSolve[∂x,x ψ[x] - κ^2 ψ[x] == 0, ψ, x] // Flatten

(* Solve the Schroedinger equation in region 2: -a<x<a. *)
(* The solution is stored in s2. The constant k is defined as k=√(2mE)/ħ *)
s2 = DSolve[∂x,x ψ[x] + k^2 ψ[x] == 0, ψ, x] // Flatten
```

Out[1]= $\{\psi \to \text{Function}[\{x\}, e^{x\kappa} c_1 + e^{-x\kappa} c_2]\}$

Out[2]= $\{\psi \to \text{Function}[\{x\}, c_1 \text{Cos}[k\, x] + c_2 \text{Sin}[k\, x]]\}$

In[3]:=

```
(* Construct the wavefunctions and define the appropriate integration constants
   in the various regions. *)

(* In region 1, we must ensure that the wavefunction remains finite for all x
   and as a result C[2] must be zero. *)
ps1 = ψ[x] /. s13 /. {C[1] → A1, C[2] → B1} /. B1 → 0

(* In region 3, we must ensure that the wavefunction remains finite for all x
   and as a result C[1] must be zero.  *)
ps3 = ψ[x] /. s13 /. {C[1] → A3, C[2] → B3} /. A3 → 0

(* In region 2, there are no constraints on the integration constants. *)
ps2 = ψ[x] /. s2 /. {C[1] → A2, C[2] → B2}
```

In[6]:=

```
(* A valid solution to the Schroedinger equation requires that the wavefunctions
   and their first derivatives match at x = -a and at x = a. *)

(* This matching condition will generate 4 equations that must be satisfied: eq1,
eq2, eq3, and eq4. *)

(* Equation 1: match wavefunctions at x = -a. *)
eq1 = ps1 == ps2 /. x → -a

(* Equation 2: match derivative of wavefunctions at x = -a. *)
eq2 = ∂x ps1 == ∂x ps2 /. x → -a

(* Equation 3: match wavefunctions at x = a. *)
eq3 = ps3 == ps2 /. x → a

(* Equation 4: match derivative of wavefunctions at x = a. *)
eq4 = ∂x ps3 == ∂x ps2 /. x → a
```

Out[6]= $A1\, e^{-a\kappa} == A2 \text{Cos}[a\, k] - B2 \text{Sin}[a\, k]$

Out[7]= $A1\, e^{-a\kappa} \kappa == B2\, k \text{Cos}[a\, k] + A2\, k \text{Sin}[a\, k]$

Out[8]= $B3\, e^{-a\kappa} == A2 \text{Cos}[a\, k] + B2 \text{Sin}[a\, k]$

Out[9]= $-B3\, e^{-a\kappa} \kappa == B2\, k \text{Cos}[a\, k] - A2\, k \text{Sin}[a\, k]$

In[10]:= (* These four equations can be combined and written in the following way:

$$\begin{pmatrix} . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \end{pmatrix} \begin{pmatrix} A1 \\ A2 \\ B2 \\ B3 \end{pmatrix} = 0$$

Solving the Schrödinger Equation using Mathematica.

```
   There is a non-trivial solution to this equation if the determinant of the
   matrix is equal to 0.
*)

(* Construct the determinant of the matrix. *)
det1 =
 Map[Coefficient[({eq1, eq2, eq3, eq4} /. Equal[a_, b_] :> a - b), #] &, {A1, A2, B2, B3}] //
    Transpose // Det // Simplify

(* Determine when the determinant is equal to 0.
 The solutions are stored in the spectral array. *)
spectral = MapAll[PowerExpand[#] &, Simplify[Flatten[Solve[det1 == 0, κ]]]] // FullSimplify

(* Determine the coefficients of the wavefunction for the first solution. *)
sol1 = Solve[{eq1, eq2, eq3, eq4} /. spectral[[1]], {A1, B2, A2, B3}] // Simplify // Flatten

(* Determine the coefficients of the wavefunction for the second solution. *)
sol2 = Solve[{eq1, eq2, eq3, eq4} /. spectral[[2]], {A1, A2, B2, B3}] // Simplify // Flatten
```

Out[10]= $e^{-2 a \kappa}\left(2 k \kappa \operatorname{Cos}[2 a k] + \left(-k^2+\kappa^2\right) \operatorname{Sin}[2 a k]\right)$

Out[11]= $\{\kappa \to -k \operatorname{Cot}[a k],\ \kappa \to k \operatorname{Tan}[a k]\}$

Out[12]= $\left\{B2 \to -A1\, e^{a k \operatorname{Cot}[a k]} \operatorname{Csc}[a k],\ A2 \to 0,\ B3 \to -A1\right\}$

Out[13]= $\left\{A2 \to A1\, e^{-a k \operatorname{Tan}[a k]} \operatorname{Sec}[a k],\ B2 \to 0,\ B3 \to A1\right\}$

```
In[14]:= (* In each region we obtain two solutions:
   one symmetric and one asyymetric solution.
 *)
```


```
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   one symmetric and one asyymetric solution.
 *)
```


```
(* Start with region 1: x < -a *)
ψ1a = ps1 /. sol1 /. spectral[[1]]
ψ1s = ps1 /. sol2 /. spectral[[2]]

(* Continue with region 2: -a < x < a *)
ψ2a = ps2 /. sol1 /. spectral[[1]]
ψ2s = ps2 /. sol2 /. spectral[[2]]

(* Finish with region 3: a < x *)
ψ3a = ps3 /. sol1 /. spectral[[1]]
ψ3s = ps3 /. sol2 /. spectral[[2]]
```

Out[14]= $A1\, e^{-k x \operatorname{Cot}[a k]}$

Out[15]= $A1\, e^{k x \operatorname{Tan}[a k]}$

Out[16]= $-A1\, e^{a k \operatorname{Cot}[a k]} \operatorname{Csc}[a k] \operatorname{Sin}[k x]$

Out[17]= $A1\, e^{-a k \operatorname{Tan}[a k]} \operatorname{Cos}[k x] \operatorname{Sec}[a k]$

Out[18]= $-A1\, e^{k x \operatorname{Cot}[a k]}$

Out[19]= $A1\, e^{-k x \operatorname{Tan}[a k]}$

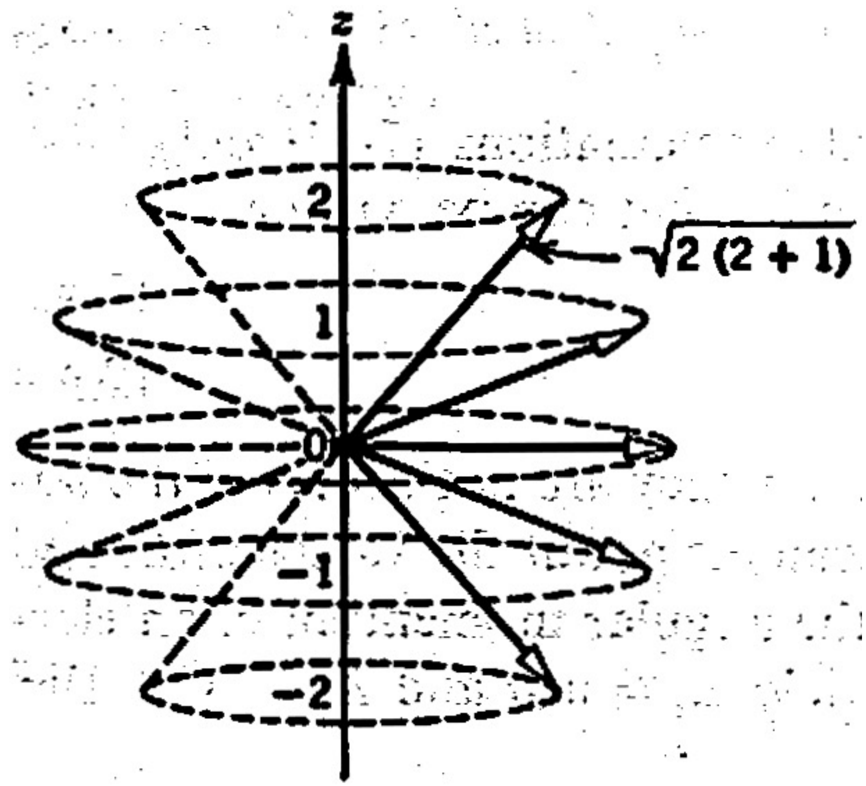
In[20]:=

Screenshot

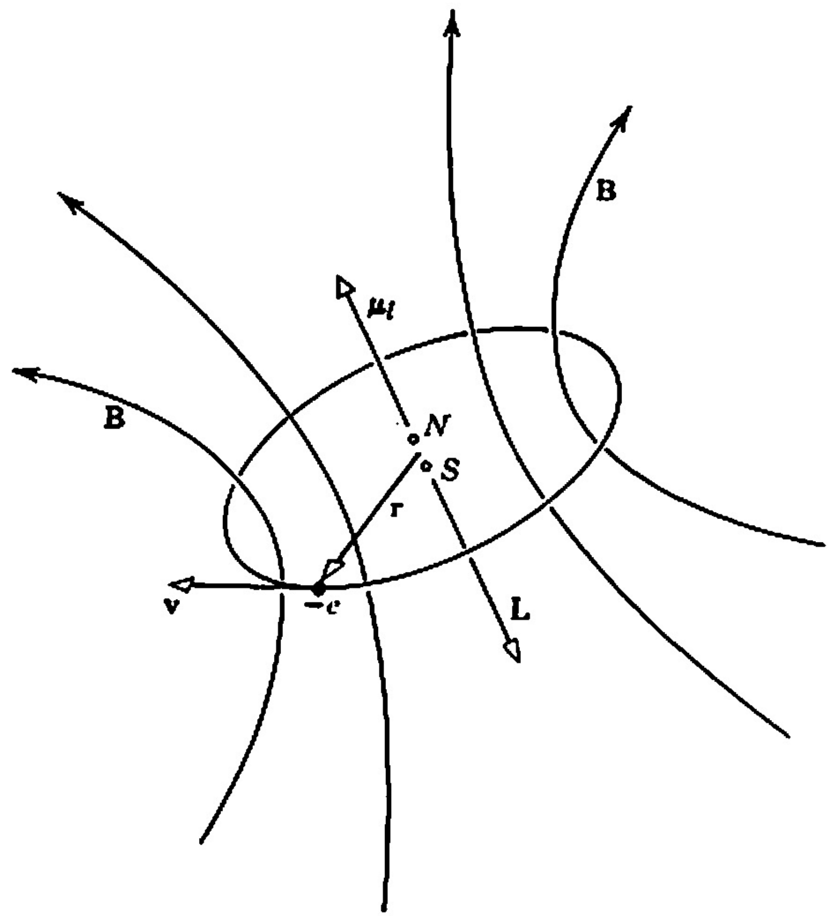
Final Comments on Spherical Symmetry.

Table 7-2 Some Eigenfunctions for the One-Electron Atom

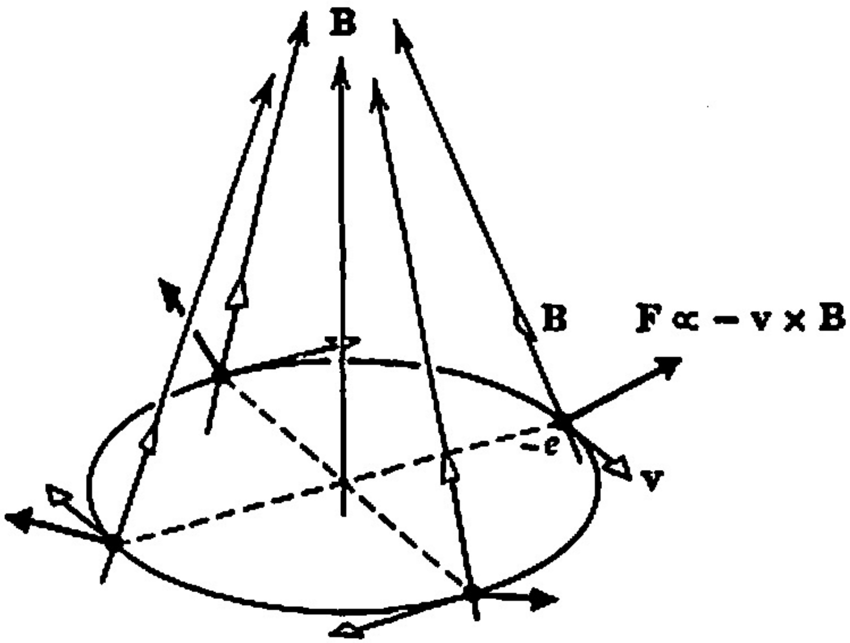
Quantum Numbers n	l	m_l	Eigenfunctions
1	0	0	$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
2	0	0	$\psi_{200} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$
2	1	0	$\psi_{210} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-Zr/2a_0}\cos\theta$
2	1	±1	$\psi_{21\pm1} = \frac{1}{8\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-Zr/2a_0}\sin\theta\, e^{\pm i\varphi}$
3	0	0	$\psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(27-18\frac{Zr}{a_0}+2\frac{Z^2r^2}{a_0^2}\right)e^{-Zr/3a_0}$
3	1	0	$\psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6-\frac{Zr}{a_0}\right)\frac{Zr}{a_0}e^{-Zr/3a_0}\cos\theta$
3	1	±1	$\psi_{31\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6-\frac{Zr}{a_0}\right)\frac{Zr}{a_0}e^{-Zr/3a_0}\sin\theta\, e^{\pm i\varphi}$
3	2	0	$\psi_{320} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2}e^{-Zr/3a_0}(3\cos^2\theta-1)$
3	2	±1	$\psi_{32\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2}e^{-Zr/3a_0}\sin\theta\cos\theta\, e^{\pm i\varphi}$
3	2	±2	$\psi_{32\pm2} = \frac{1}{162\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2}e^{-Zr/3a_0}\sin^2\theta\, e^{\pm 2i\varphi}$

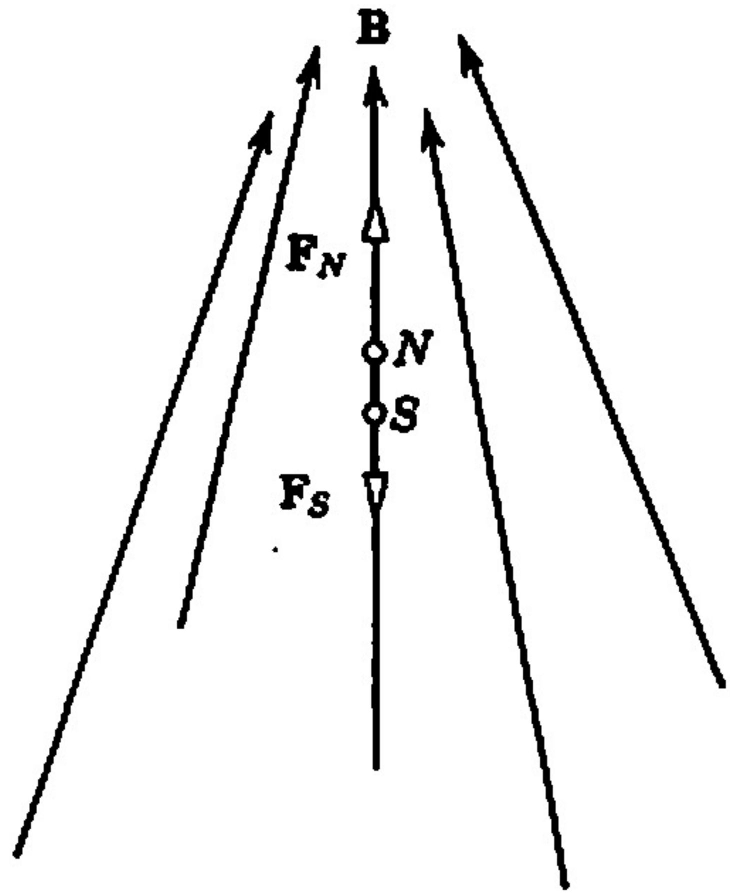


Chapter 8.
An atomic electron in a magnetic field.



Forces on a magnetic dipole.

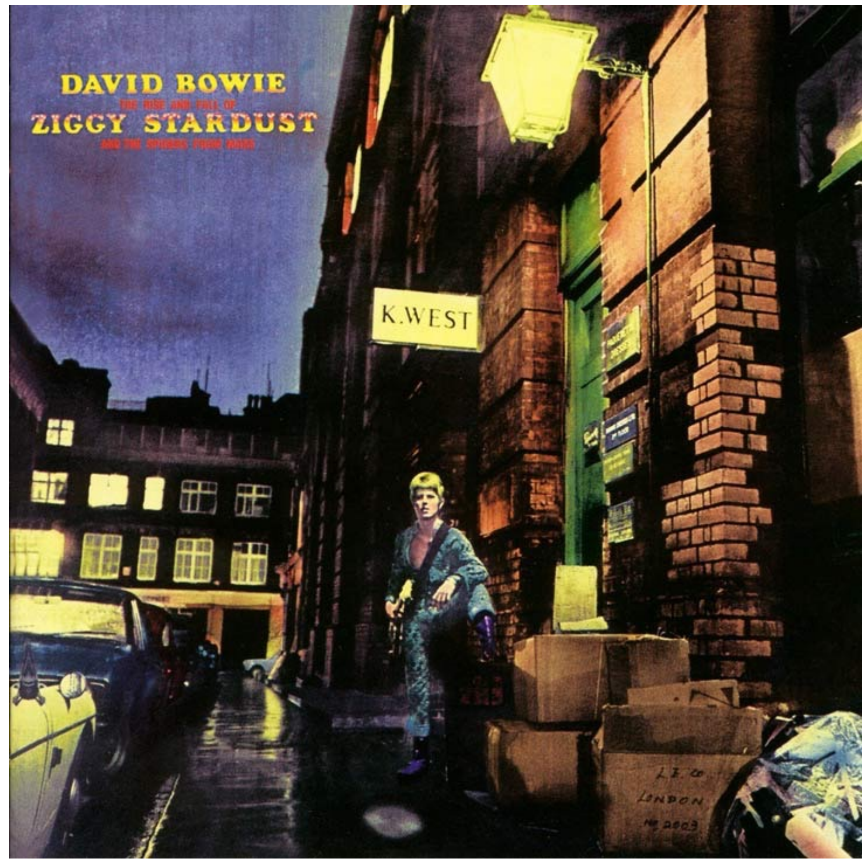




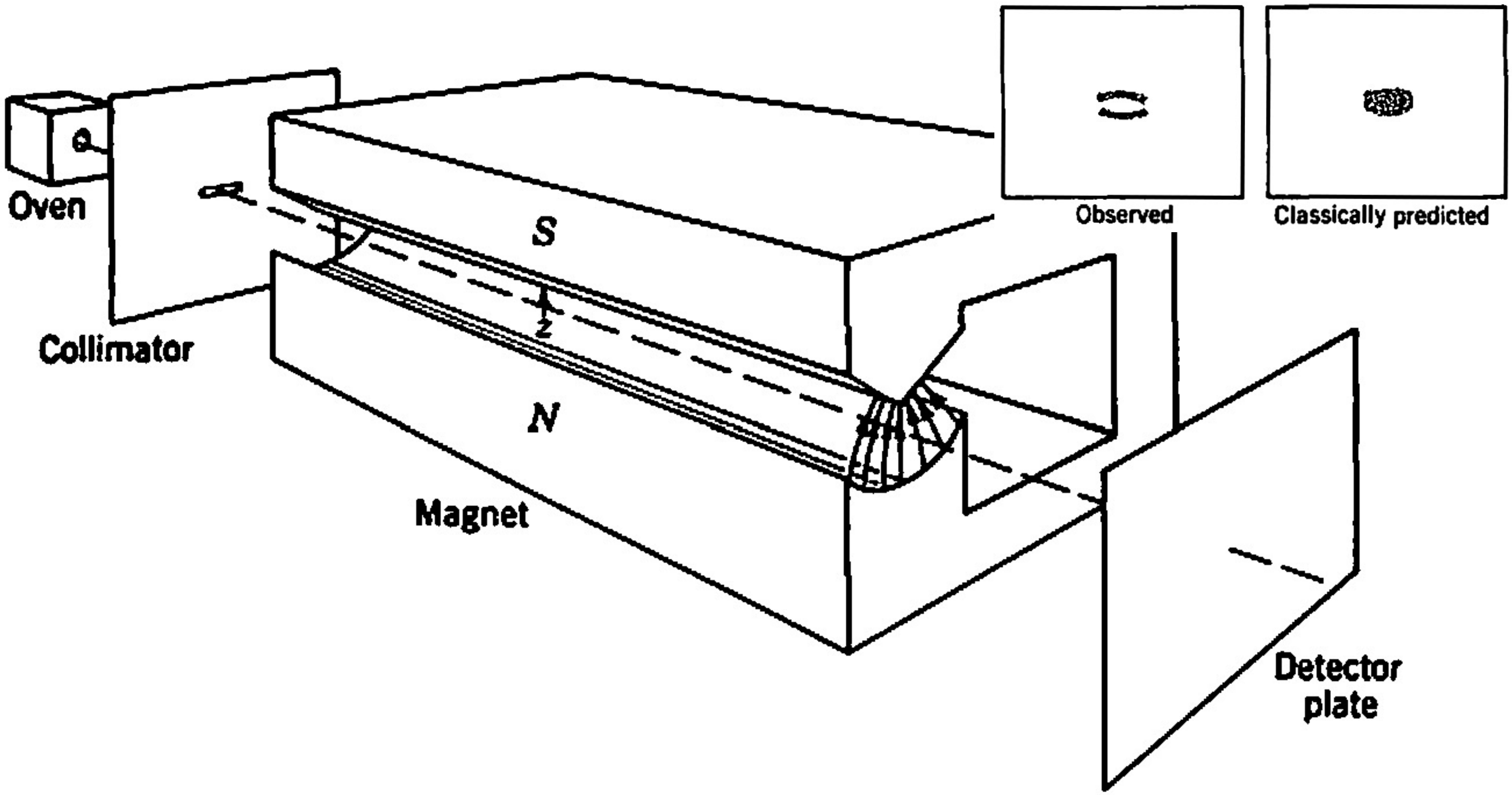
4 Minute 13 Second Intermission.

- Since paying attention for 1 hour and 15 minutes is hard when the topic is physics, let's take a 4 minute 13 second intermission.

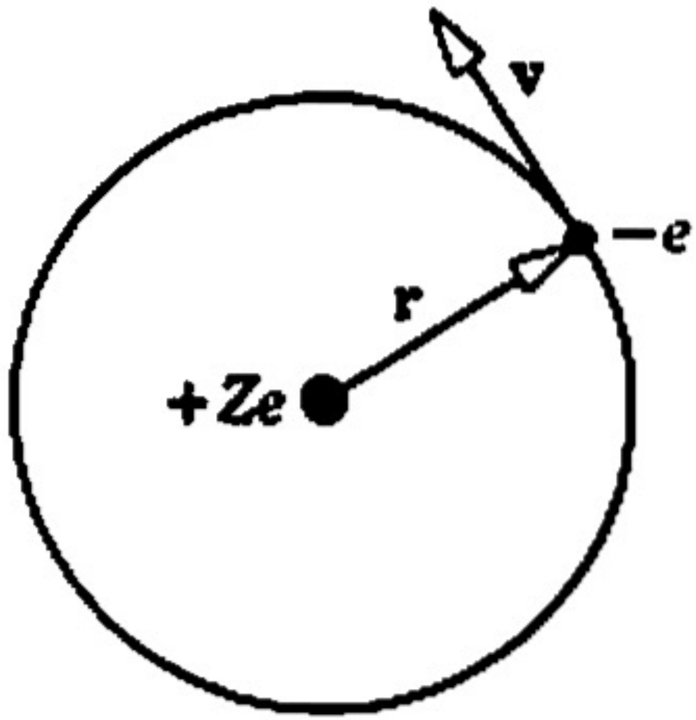
- You can:
  - Stretch out.
  - Talk to your neighbors.
  - Ask me a quick question.
  - Enjoy the fantastic music.

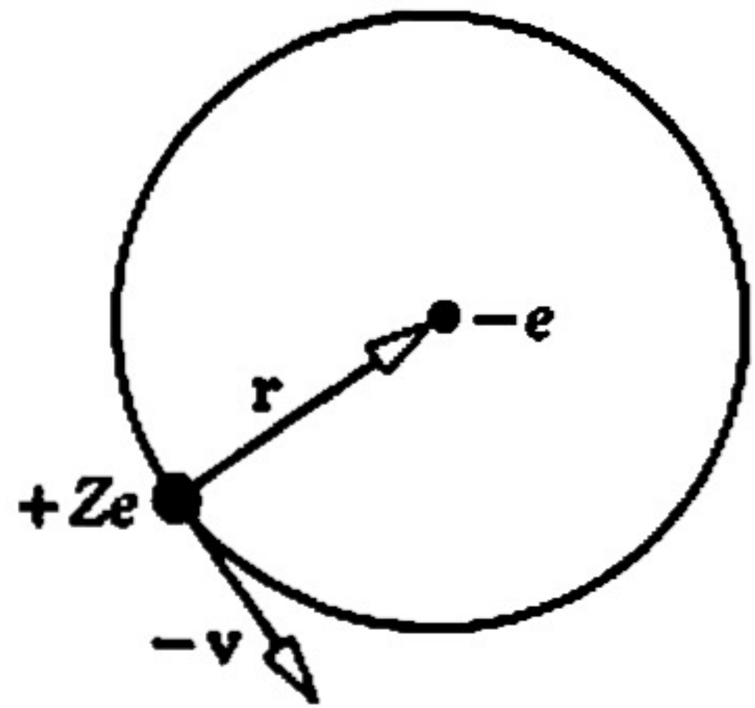


The Stern-Gerlach Experiment.



The Spin-Orbit Interaction.





ENOUGH FOR TODAY?