*IIT Madras*

Quantum Mechanics
an invitation

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In this chapter we shall tackle immediately the basic element of the mysterious behaviour in its most strange form. We choose to examine a phenomenon which is **impossible, absolutely impossible, to explain in any classical way, and which has in it the heart of quantum mechanics**. In reality, it contains the only mystery. We cannot make the mystery go away by "explaining" how it works. We will just tell you how it works. In telling you how it works we will have told you about the basic peculiarities of all quantum mechanics.
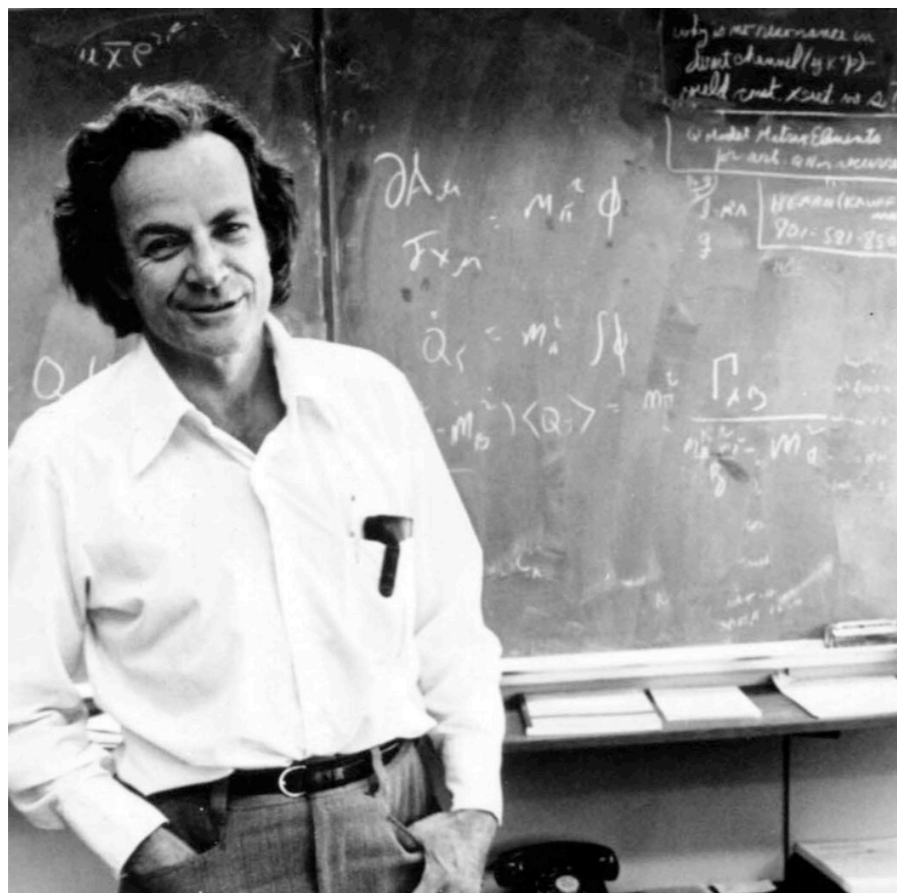
Richard Feynman

The Feynman Lectures on Physics [Vol III, Ch 1]
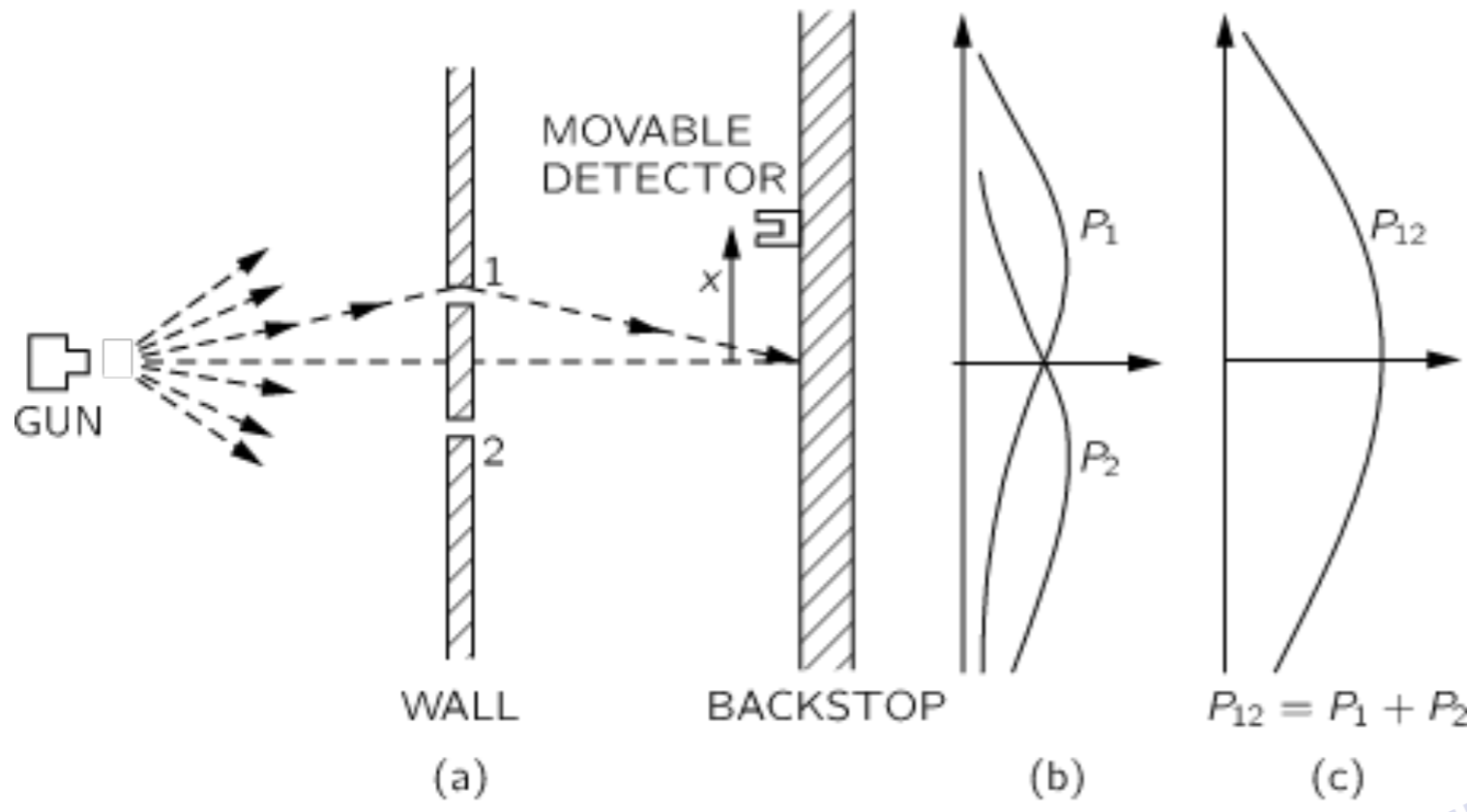
MOVABLE DETECTOR

GUN

x

1

2

WALL

BACKSTOP

P_1

P_2

P_{12}

$P_{12} = P_1 + P_2$

(a)

(b)

(c)

Double slit experiment with BULLETS

- Probability with both slits open is the **sum** of probabilities with either slit open

- This is characteristic of a *no-interference* and signifies a **particle** behaviour

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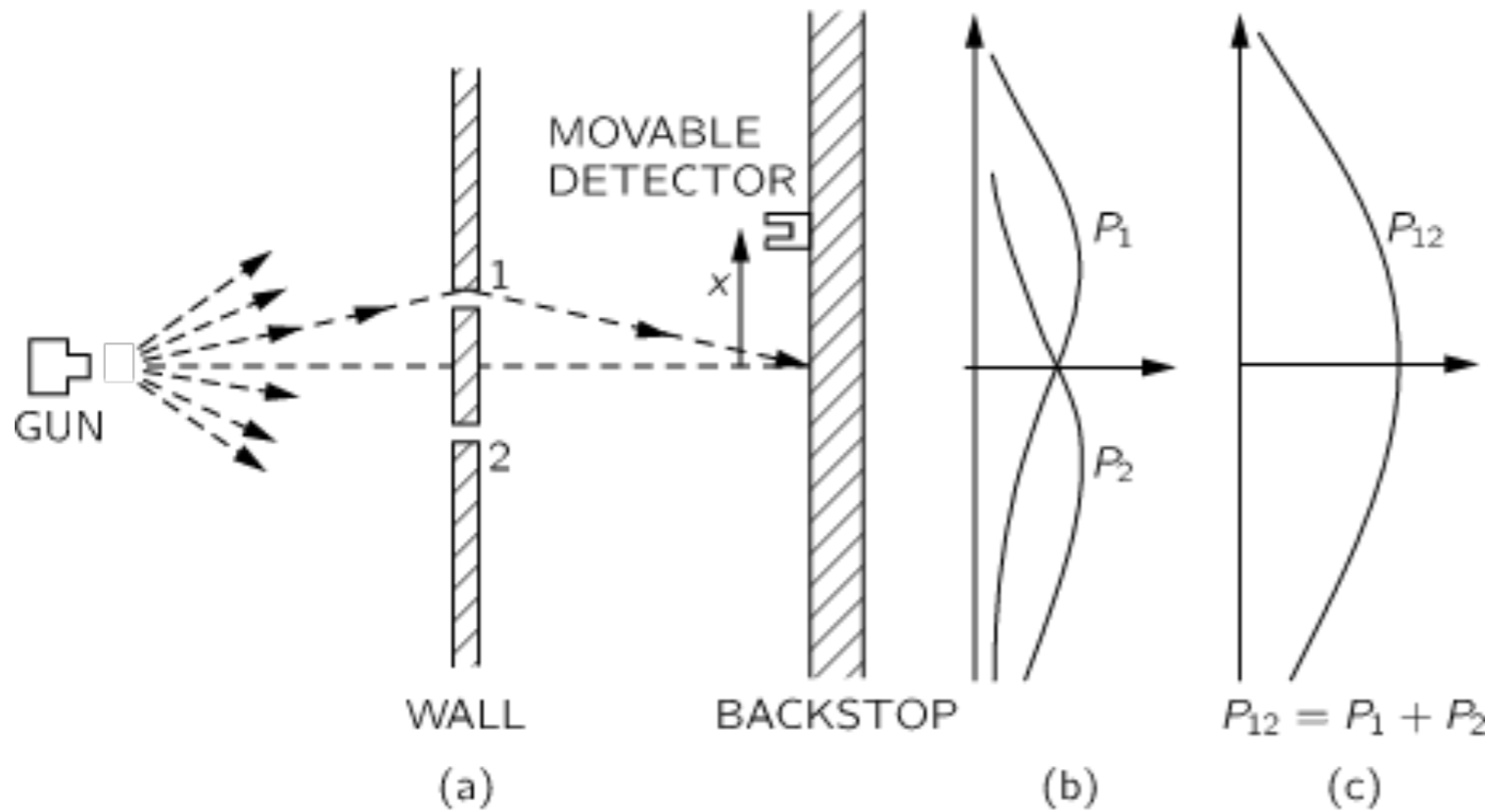
3

Double slit experiment with BULLETS

- Probability with both slits open is the **sum** of probabilities with either slit open

- This is characteristic of a *no-interference* and signifies a **particle** behaviour

Double slit experiment with WAVES

- Intensity with both slits open is **NOT** the **sum** of intensities with either slit open

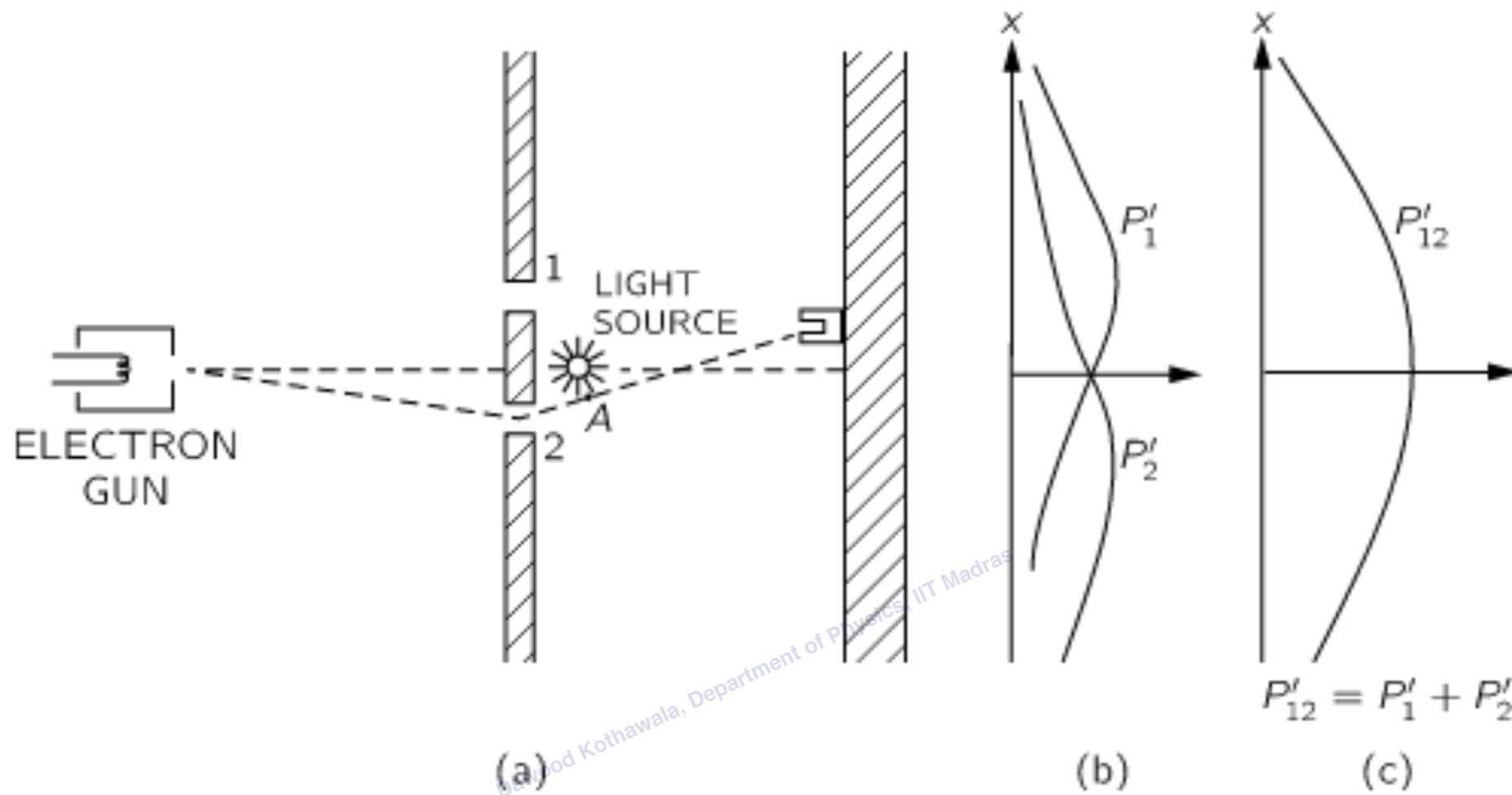- This is characteristic of an *interference* and signifies a **wave** behaviour
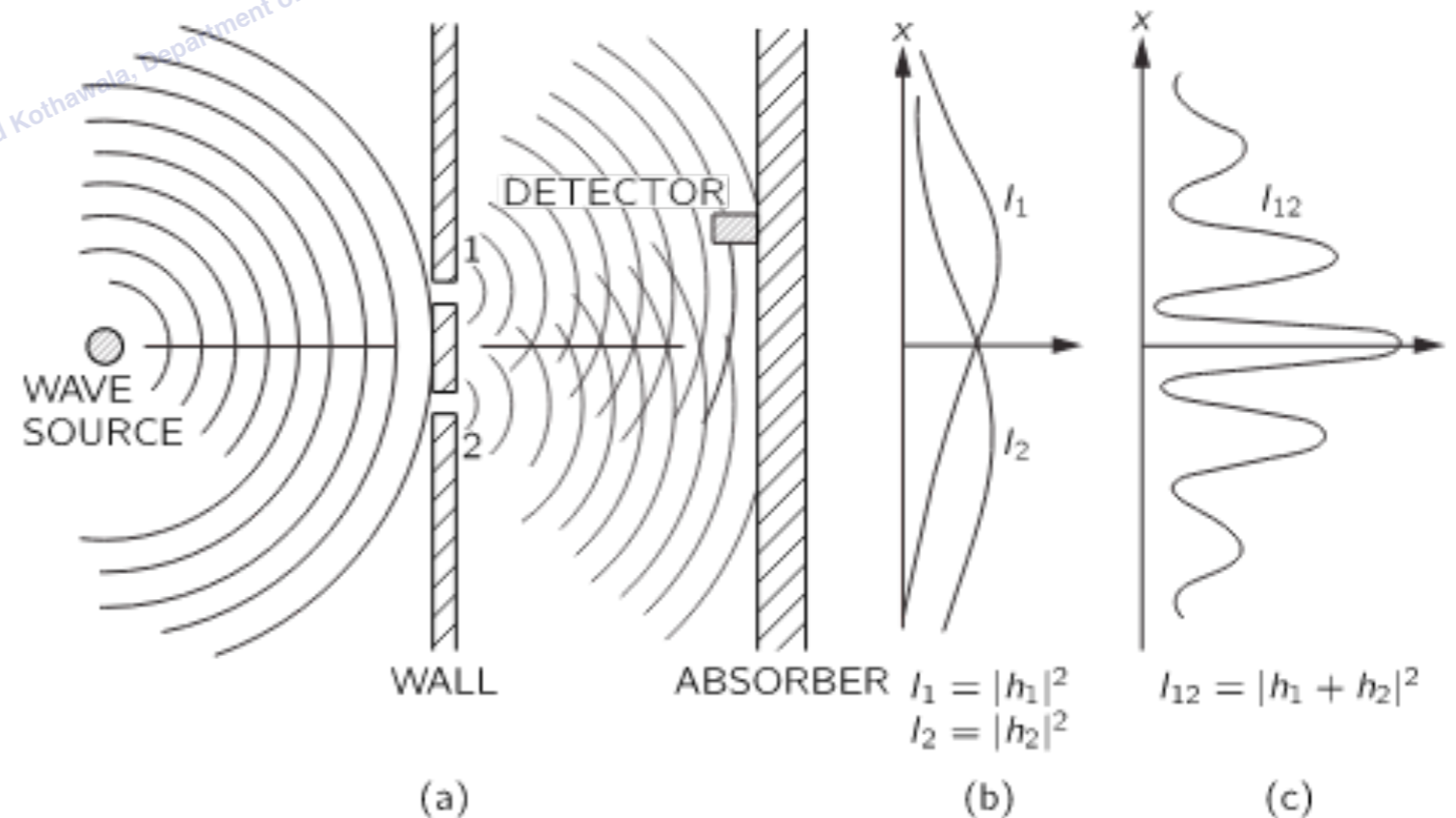
4

Double slit experiment with ELECTRONS
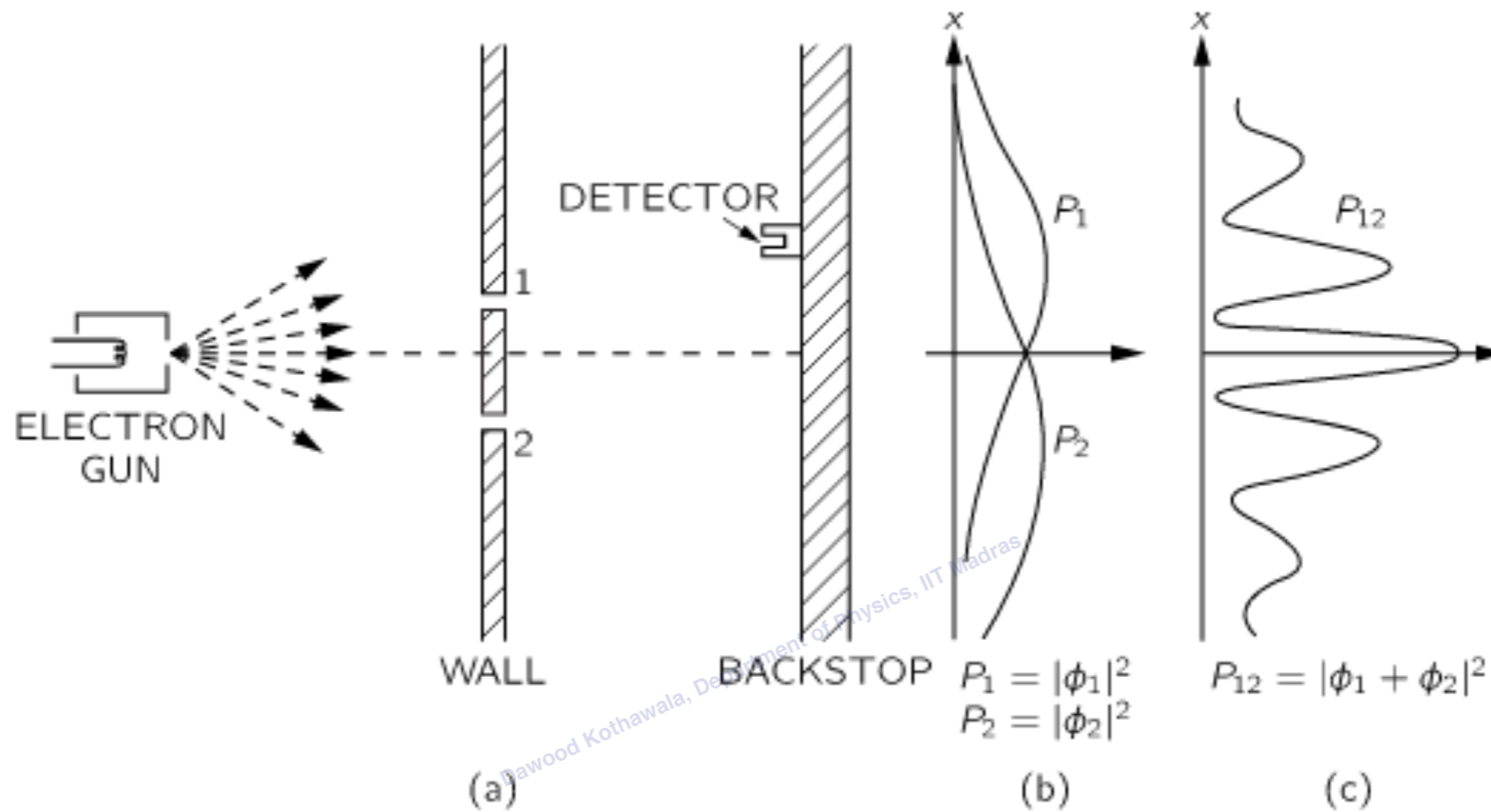
The distribution pattern is similar to that for the waves!
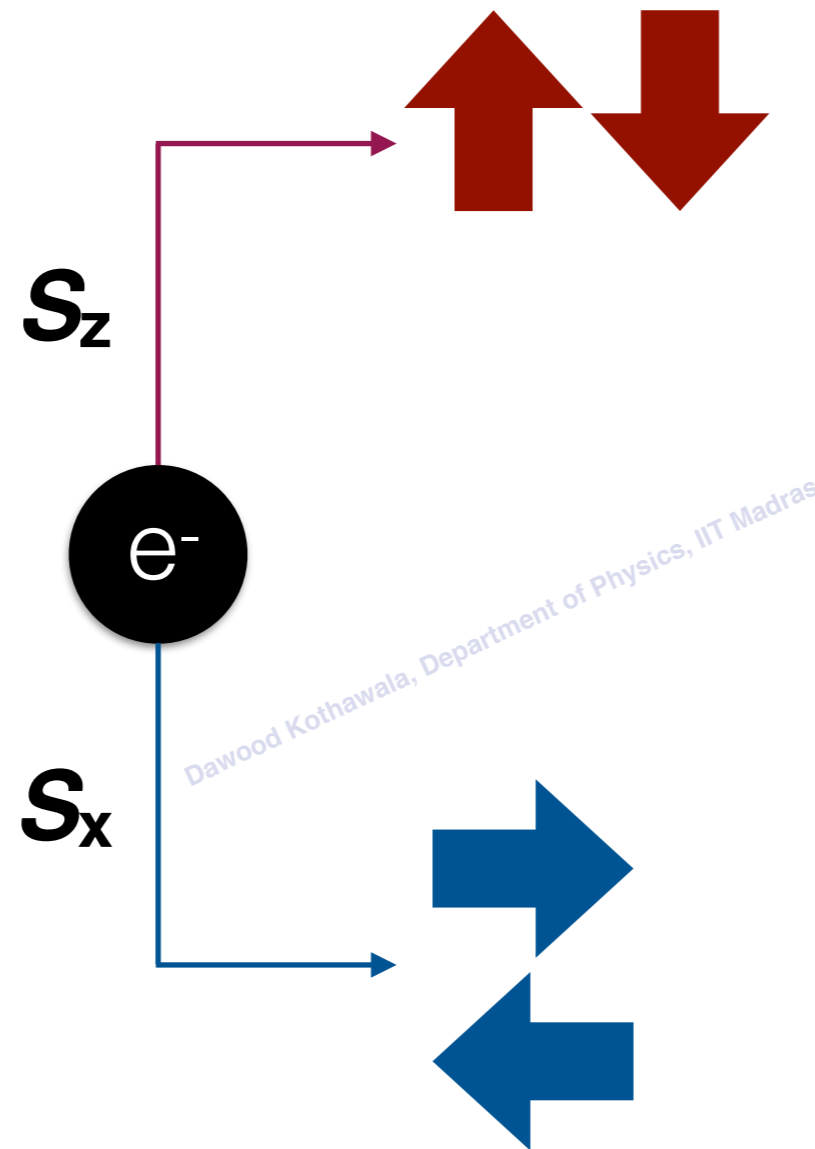
What wave?

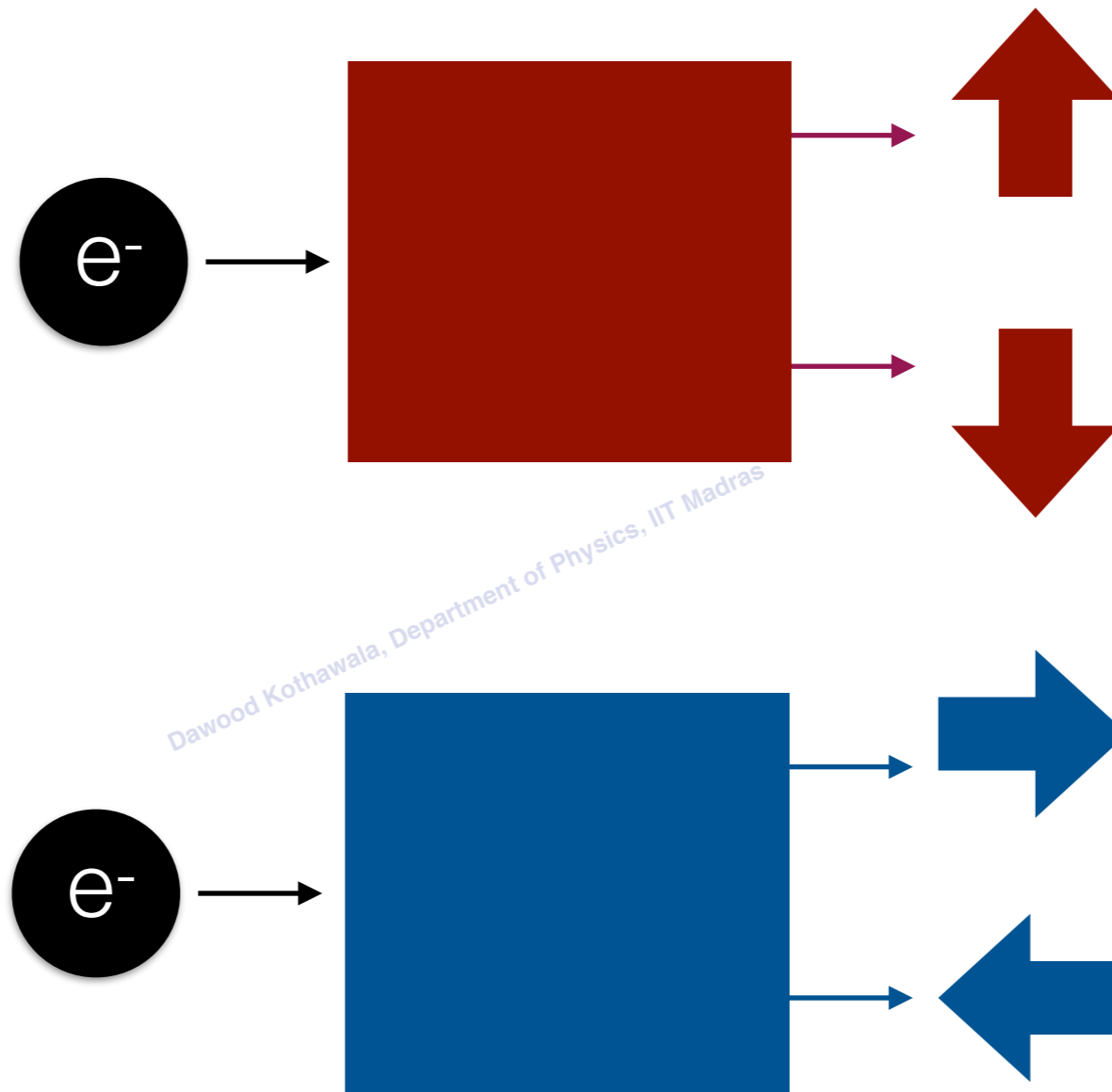# Double slit experiment with ELECTRONS

The distribution pattern is similar to that for the bullets when one tries to observe which slit the electron passes through!
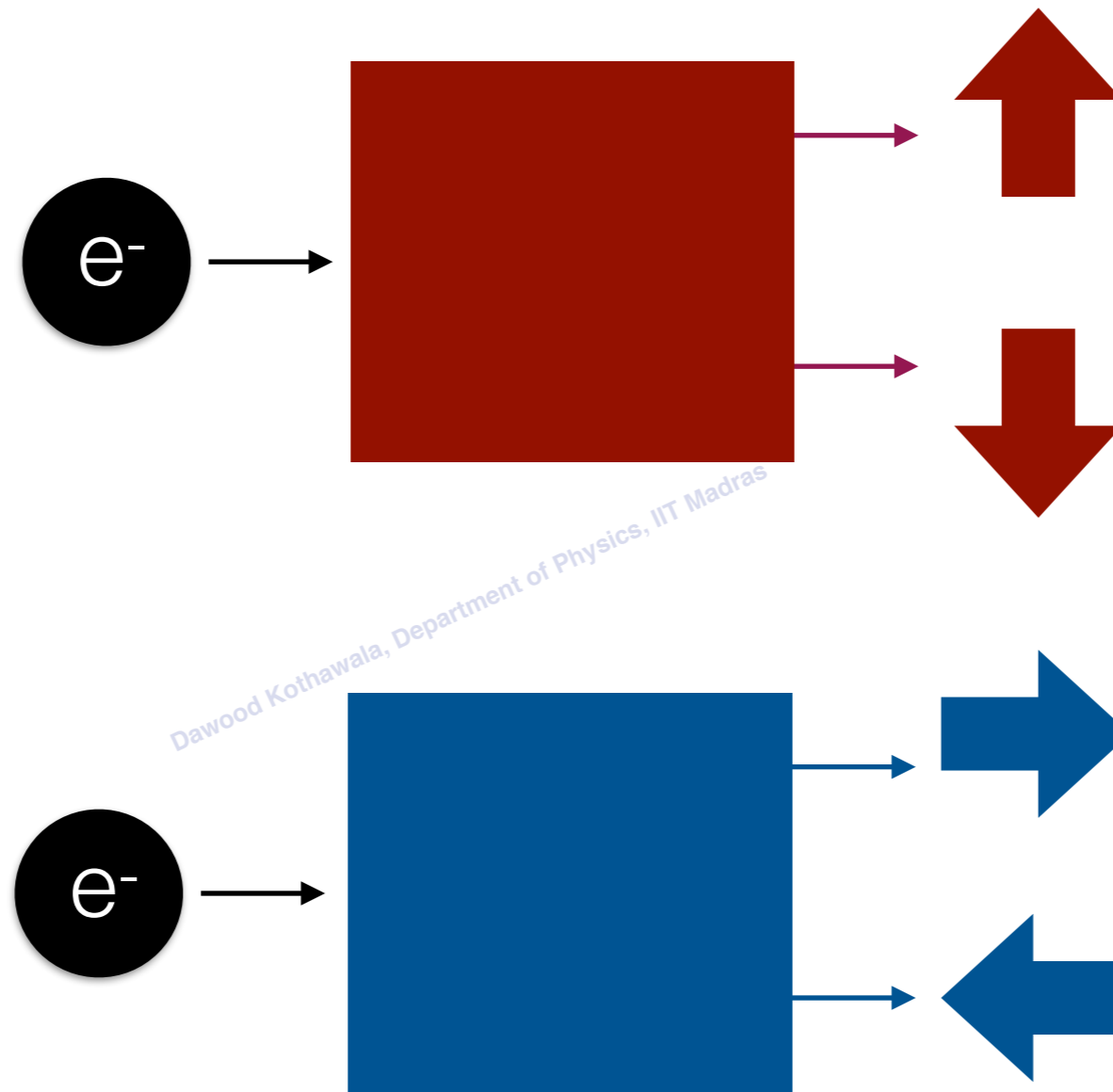
The Stern-Gerlach experiment
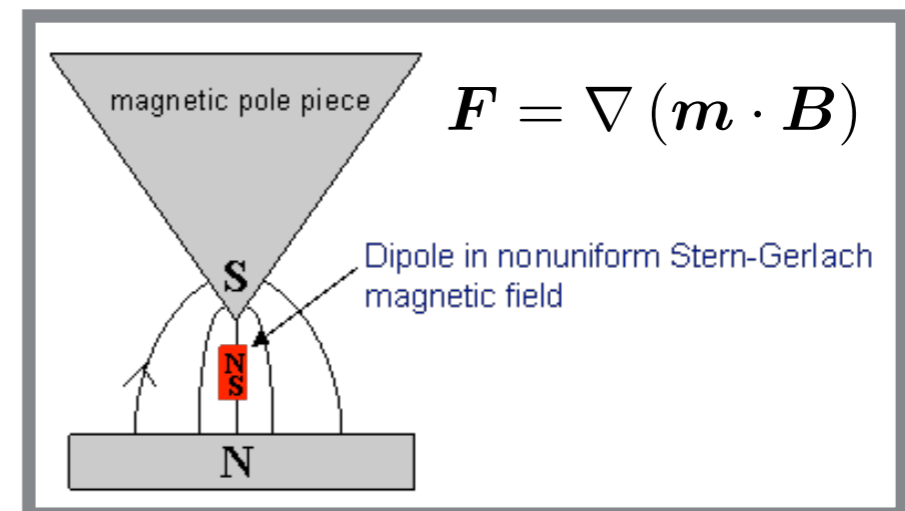
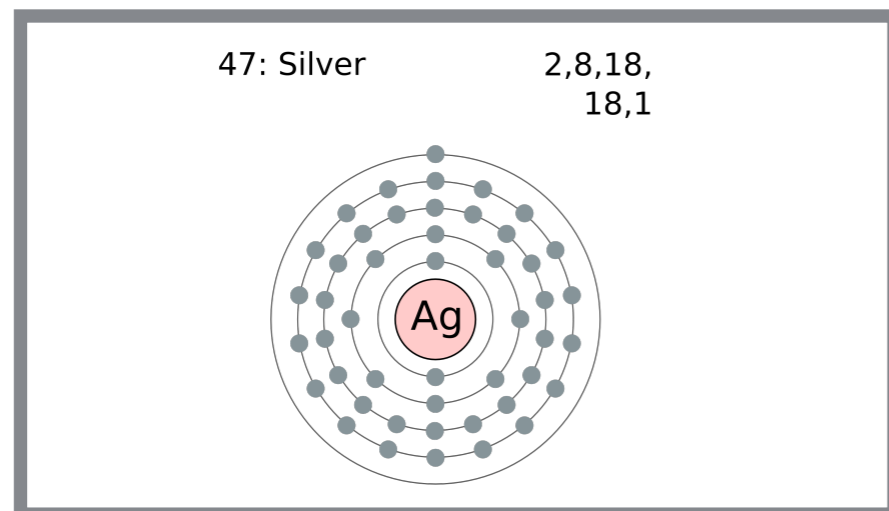S_z

S_x

e⁻

The Stern-Gerlach experiment

8

The Stern-Gerlach experiment

What's inside these boxes?

The Stern-Gerlach experiment
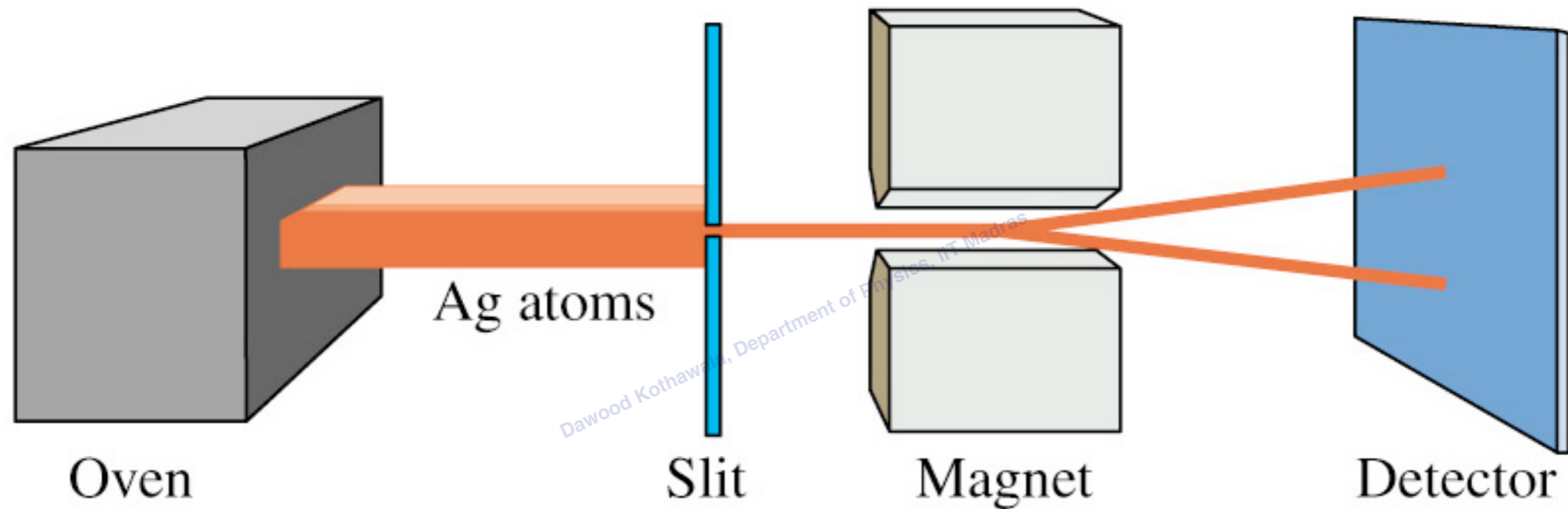
The experimental apparatus inside the box

Oven — Ag atoms — Slit — Magnet — Detector

47: Silver   2,8,18, 18,1

Ag

magnetic pole piece

$$F = \nabla\left(m \cdot B\right)$$

S

N
S

Dipole in nonuniform Stern-Gerlach magnetic field

N

The experimental apparatus inside the box

Ag atoms

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Oven
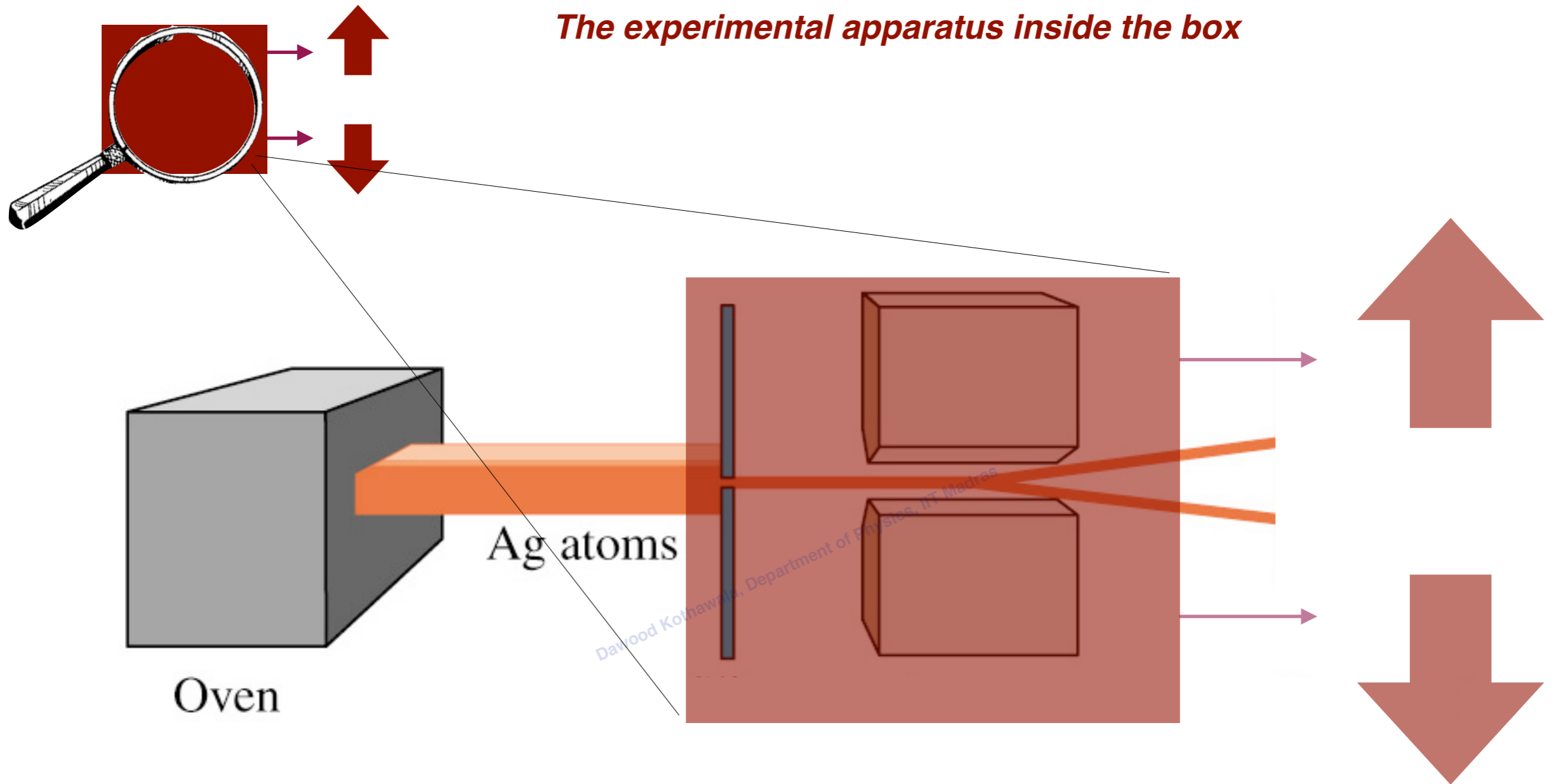
Der experimentelle Nachweis der Richtungsquantelung im Magnetfeld.

Von **Walther Gerlach** in Frankfurt a. M. und **Otto Stern** in Rostock.

Mit sieben Abbildungen. (Eingegangen am 1. März 1922.)

Fig. 2.

Fig. 3.

**THE SPIN,
A QUANTUM MAGNET**

All the animations and explanations on
www.toutestquantique.fr

The plaque shows schematically the apparatus of the experiment, and Stern (L) and Gerlach (R). The text says:

In February 1922, the fundamental discovery of the space quantisation of the magnetic moments in atoms was made in this building of the Physikalischer Verein, Frankfurt am Mai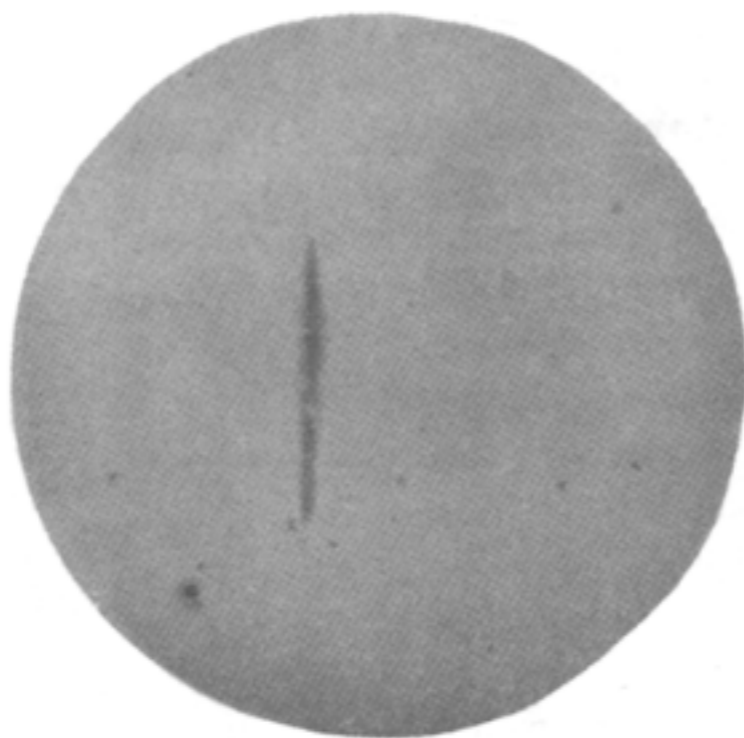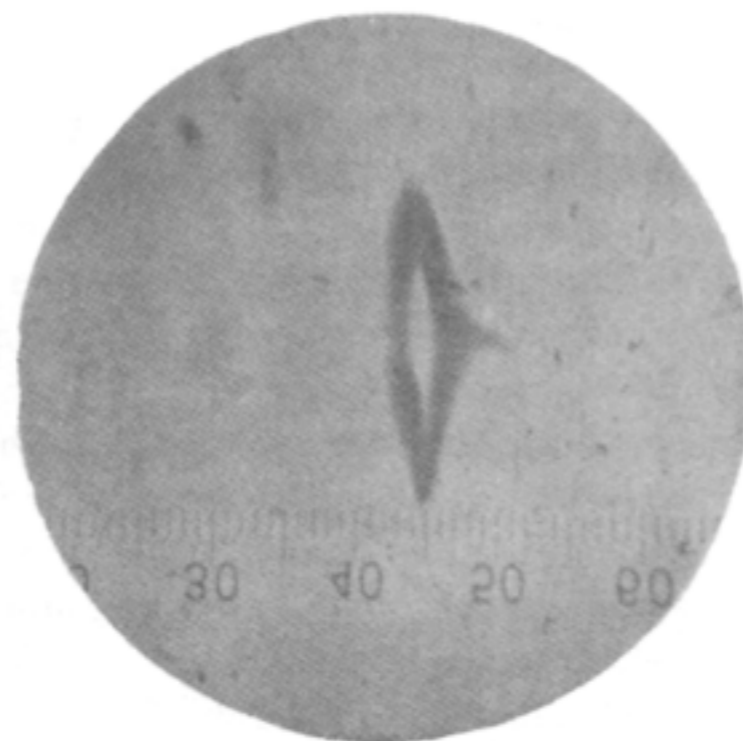n, by Otto Stern and Walther Gerlach. The Stern-Gerlach experiment is the foundation of important physical and technical developments of the 20th century, such as the nuclear resonance method, the atomic clock, or the laser. Otto Stern was awarded the Noble prize for this discovery in 1943.

The Stern-Gerlach experiment

The experimental apparatus inside the box

Ag atoms

Oven
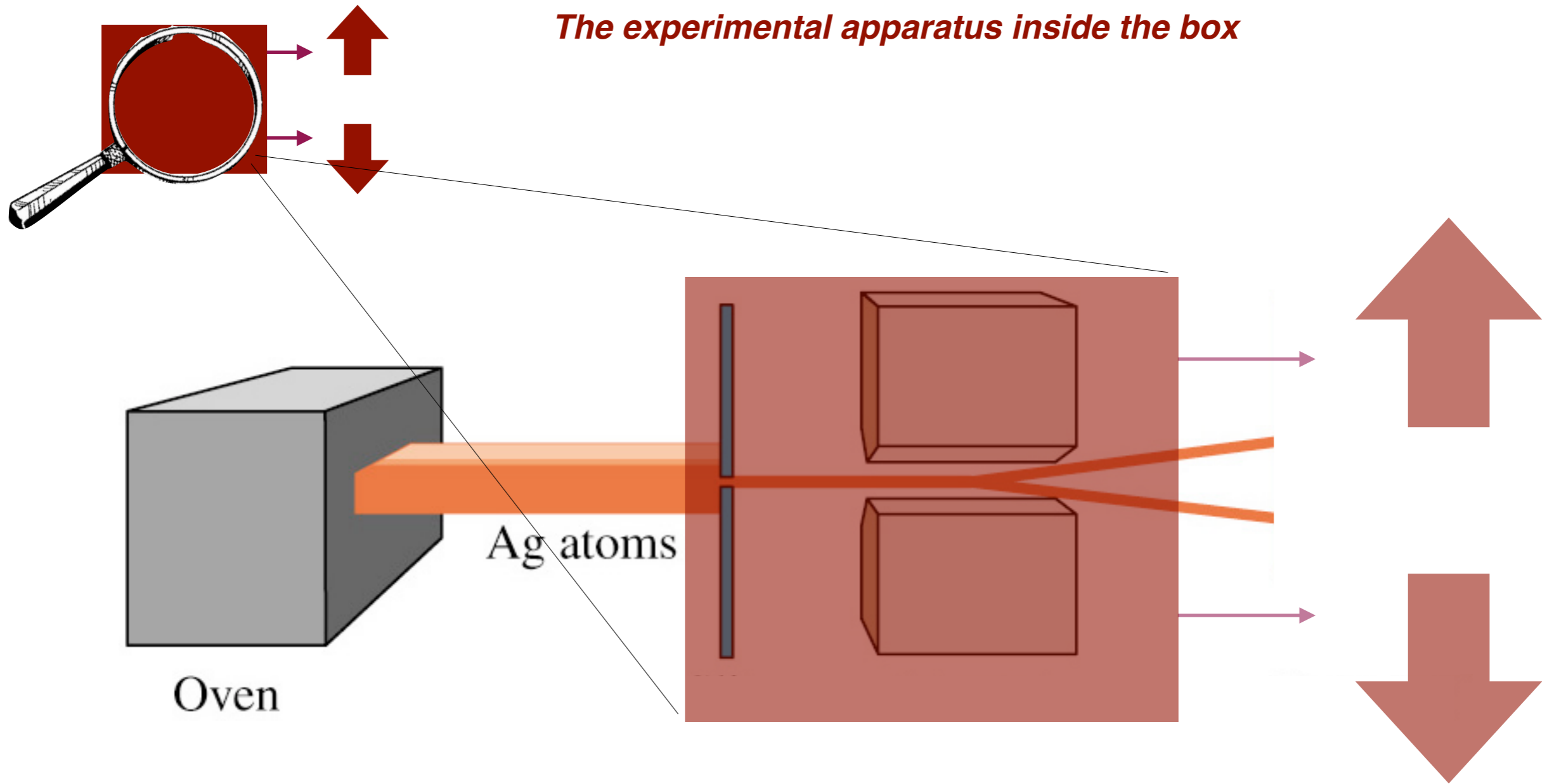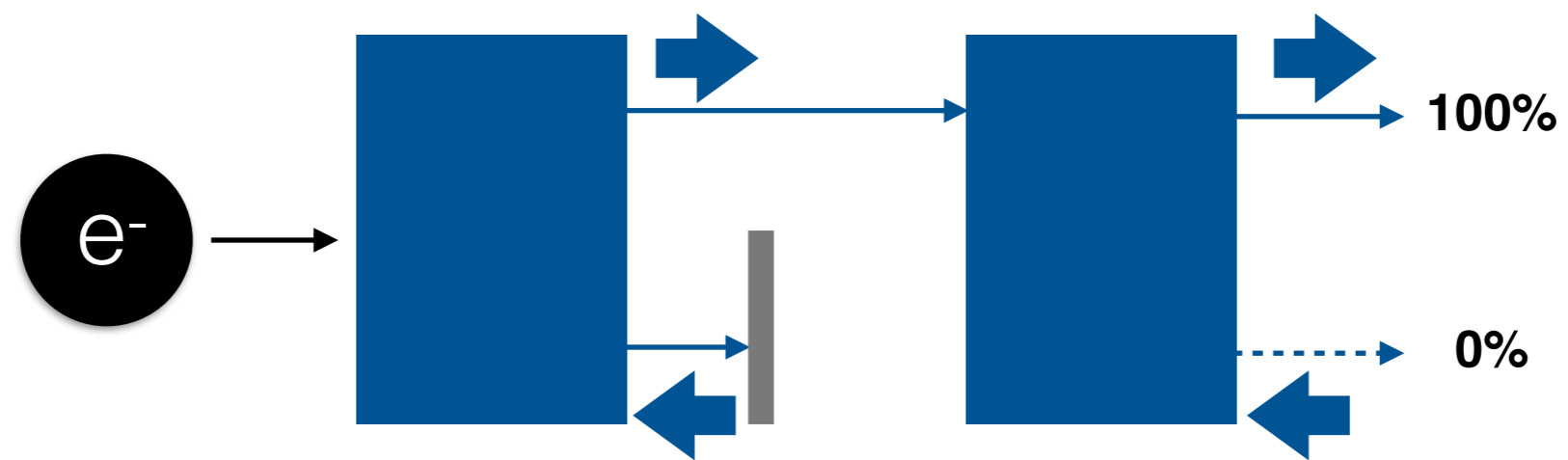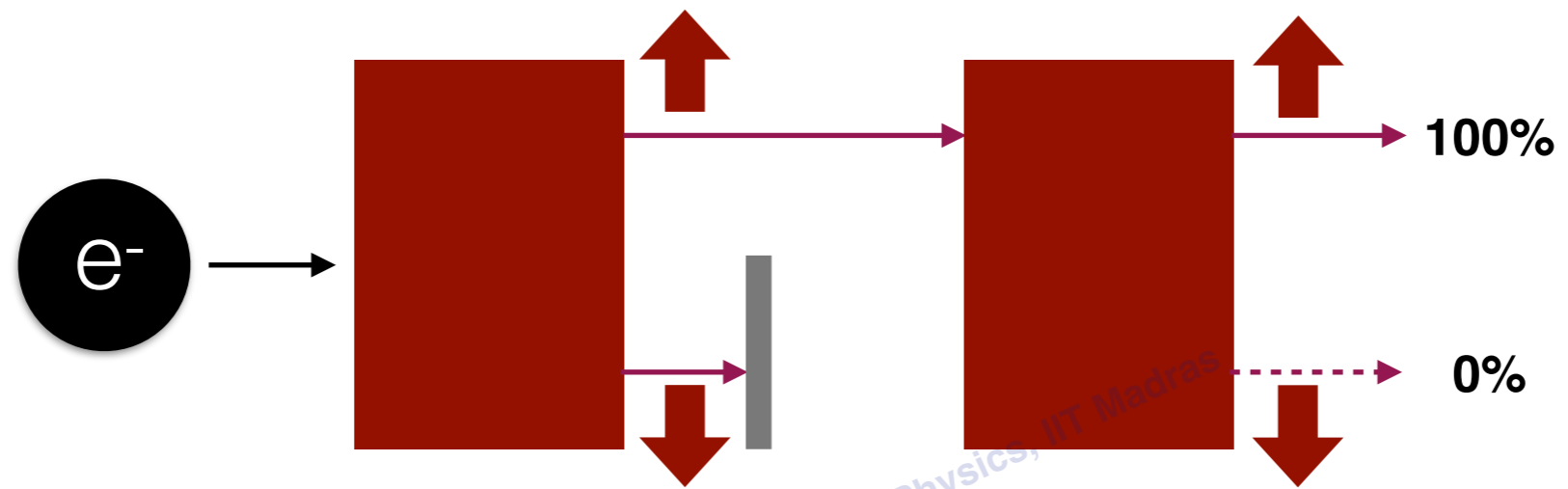
The Stern-Gerlach experiment

The Stern-Gerlach experiment

17

50%

50%

e⁻

50%

50%

50%

50%

e⁻

50%

?

?
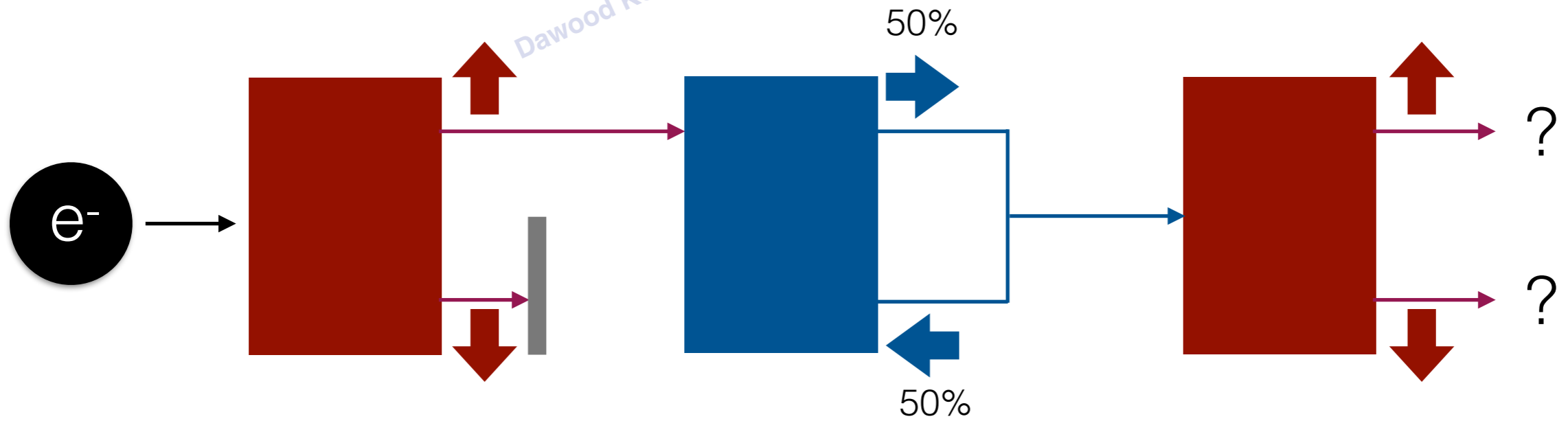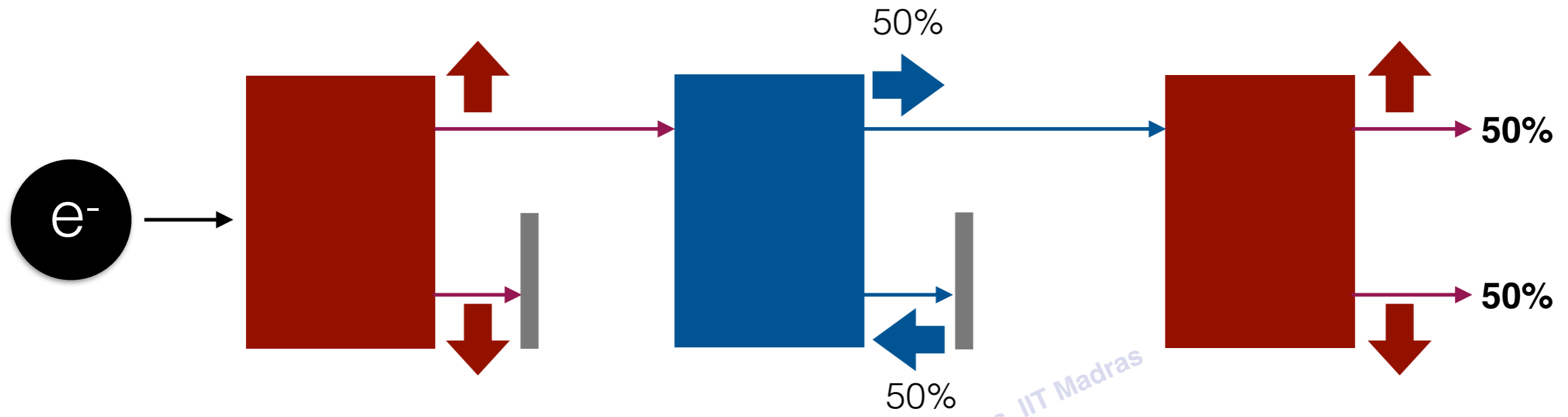
The Stern-Gerlach experiment
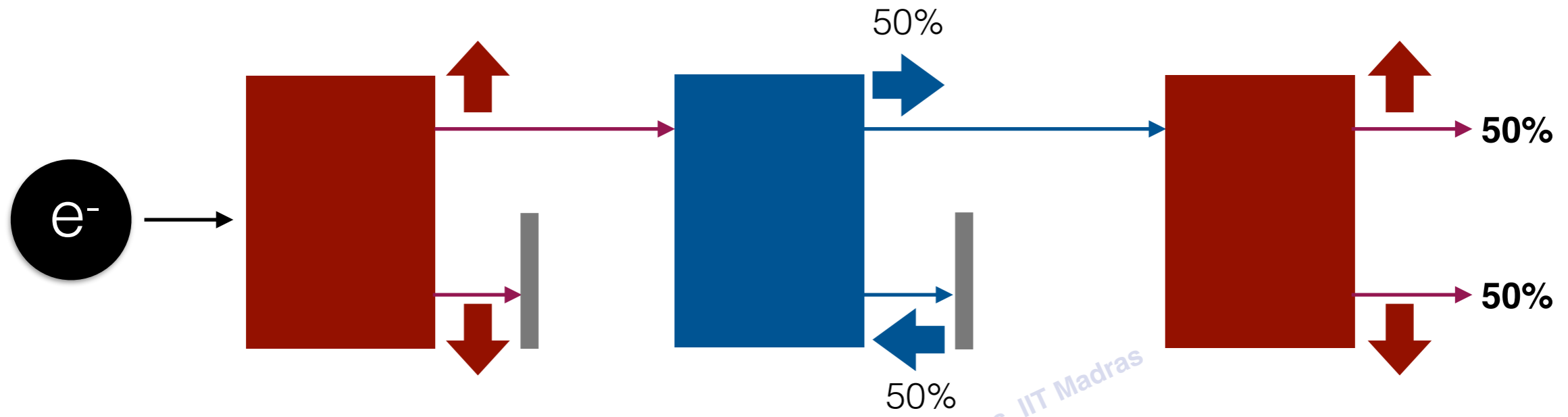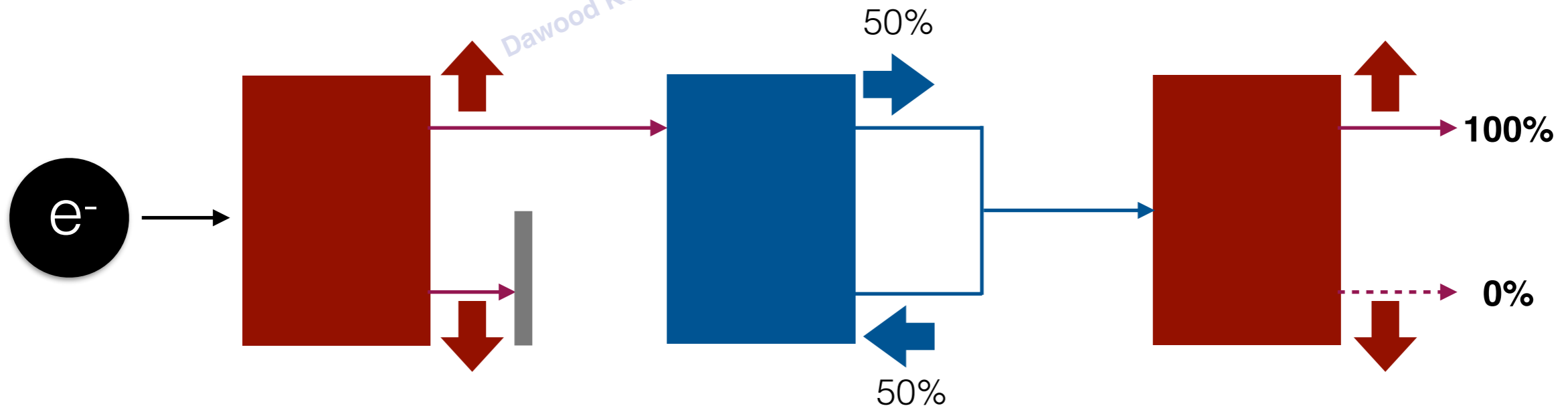
Magnetic moment takes only two possible values

This turns out to be true for many other properties, such as Energy, Angular momentum etc, for many systems

Eg: A particle in a box can have only a fixed set of energies
     A harmonic oscillator can have only a fixed set of energies
     An electron in a hydrogen atom can have only fixed set of energies

Unlike in Classical Physics, physical observables associated with a system, such as, *E, L,* may not take arbitrary values

Physical properties of a system is intimately tied to the kind of measurements made on the system. Without any such measurement, it makes no sense to talk of *a* value of a particular physical quantity*.*

*Eg: knowing the z-component of Spin of an electron wipes out any earlier information we might have had about its x-component. This is not unrelated to the **uncertainty principle**.*

This, again, is in stark contrast to what happens in Classical Physics, where a system has well defined values for observable regardless of measurement

$$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}$$

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\psi(\mathbf{r},t)$$

(Schrodinger equation)

$$\mathbf{r}(t)$$
$$\mathbf{v}(t)$$

$$\boxed{\psi(\mathbf{r},t)}$$

*This is called the **wave function** of a system. It is in general a **complex** function.*

$$\mathbf{r}(t) \longrightarrow \widehat{\mathbf{r}}$$

$$\mathbf{v}(t) \longrightarrow \widehat{\mathbf{p}}$$

$$\psi(\mathbf{r}, t) \to P(\mathbf{r}, t) = \psi^* \psi$$

probability density

$$\mathbf{r}(t) \longrightarrow \widehat{\mathbf{r}}$$

$$\mathbf{v}(t) \longrightarrow \widehat{\mathbf{p}}$$
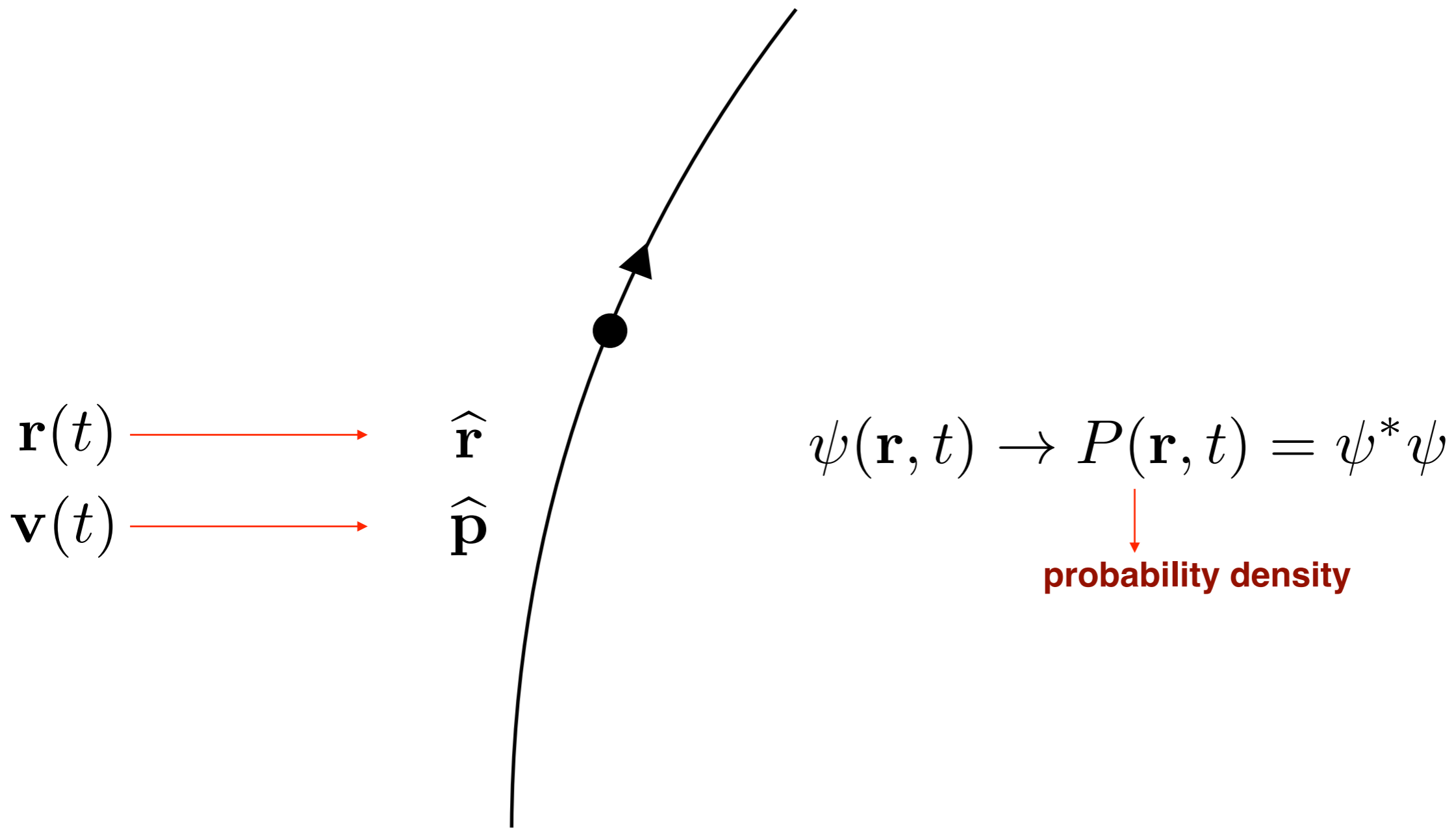
$$\psi(\mathbf{r}, t) \rightarrow P(\mathbf{r}, t) = \psi^*\psi$$

probability density

$$\int \psi^*\psi \, d^3\mathbf{r} = \int P(\mathbf{r}, t) \, d^3\mathbf{r} = 1$$

$$\mathbf{r}(t) \longrightarrow \widehat{\mathbf{r}}$$

$$\mathbf{v}(t) \longrightarrow \widehat{\mathbf{p}}$$
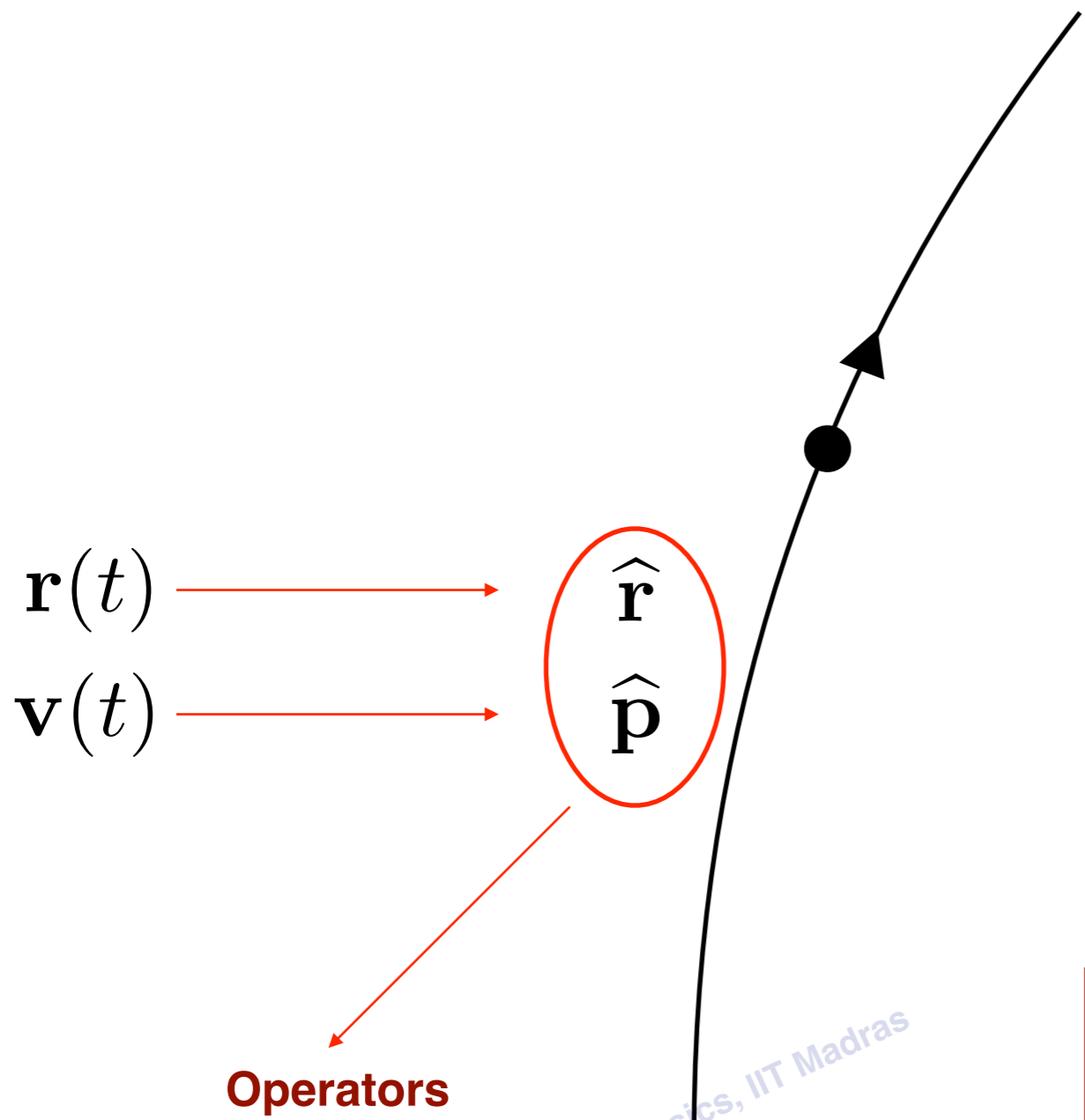
Operators

$$\psi(\mathbf{r}, t) \rightarrow P(\mathbf{r}, t) = \psi^* \psi$$

probability density

$$\langle \hat{\mathbf{r}} \rangle(t) = \int d^3\mathbf{r} \; P(\mathbf{r}, t) \; \mathbf{r}$$

Operators

Input   Output

Position
operator

$$\psi(\mathbf{r}, t) \longrightarrow \boxed{\widehat{\mathbf{r}}} \longrightarrow \mathbf{r}\,\psi(\mathbf{r}, t)$$

Momentum
operator

$$\psi(\mathbf{r}, t) \longrightarrow \boxed{\widehat{\mathbf{p}}} \longrightarrow -i\hbar\nabla\psi(\mathbf{r}, t)$$

To every "observable" (eg, position, momentum) there corresponds an "operator" which acts on the wave function in a specific manner

Example: $\psi(\mathbf{r}, t) = C e^{i(\boldsymbol{k}\cdot\mathbf{r} - \omega t)}$

$$\widehat{\mathbf{r}}\,\psi = \mathbf{r}\psi$$

$$\widehat{\mathbf{p}}\,\psi = (\hbar\boldsymbol{k})\,\psi$$

The above definitions of position and momentum operators therefore make perfect sense

$$H = \frac{p^2}{2m} + V(\mathbf{r}, t)$$

time evolution operator

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \psi(\mathbf{r}, t)$$
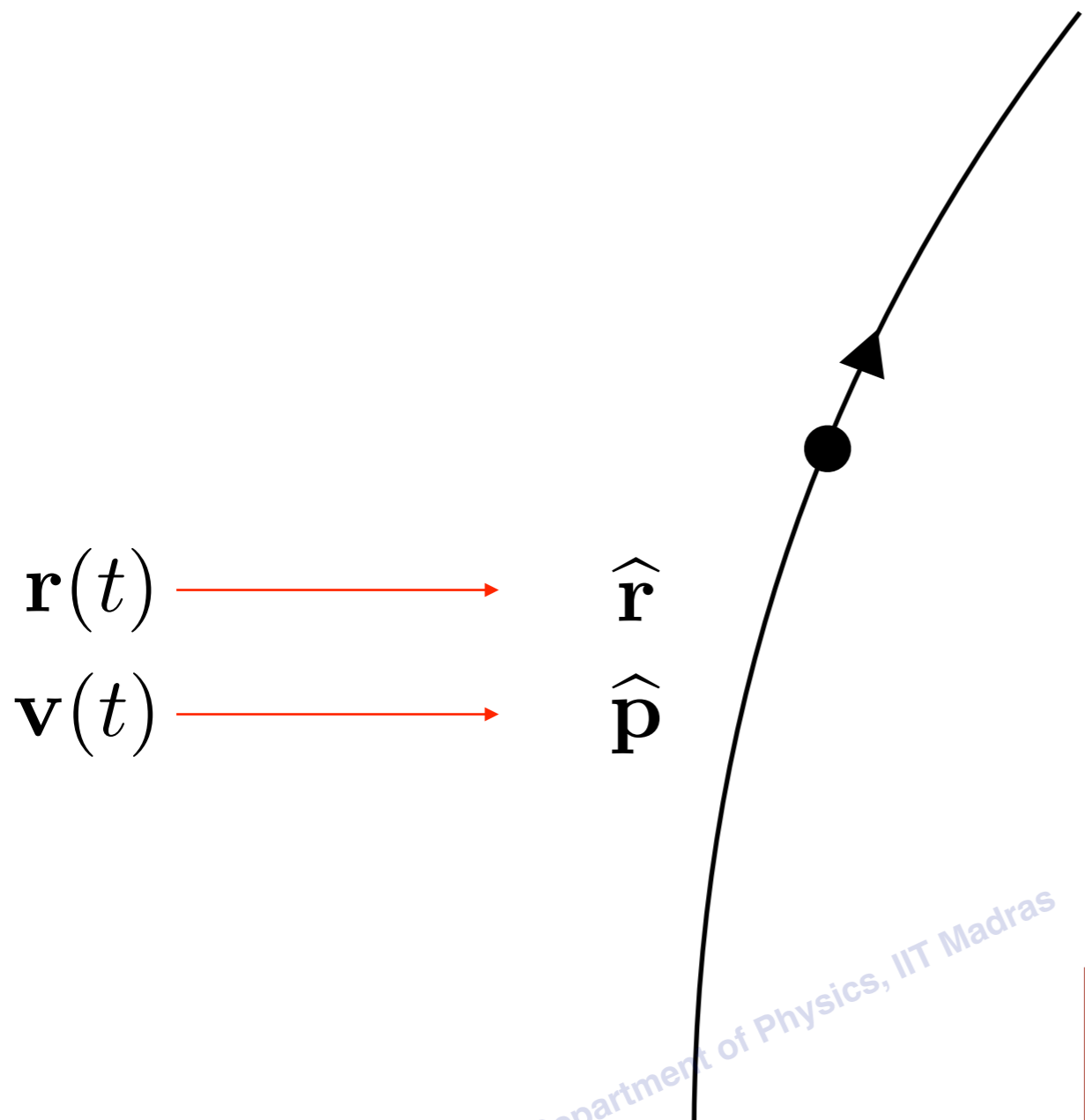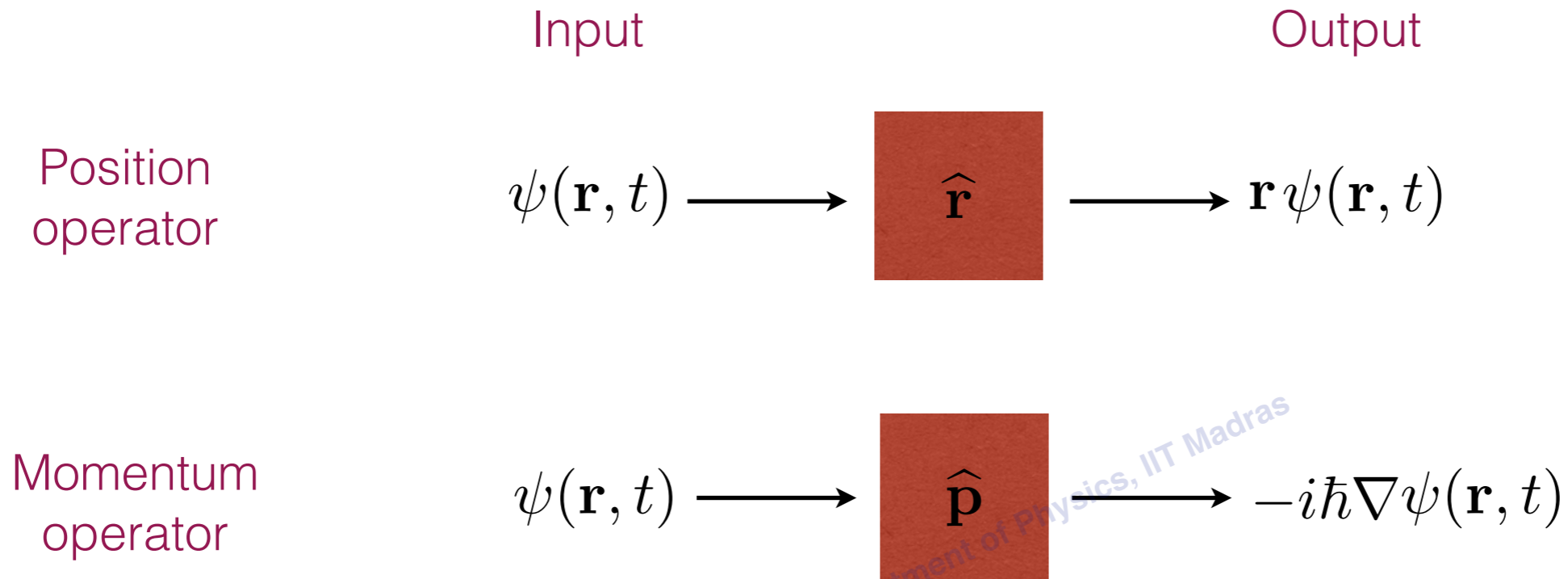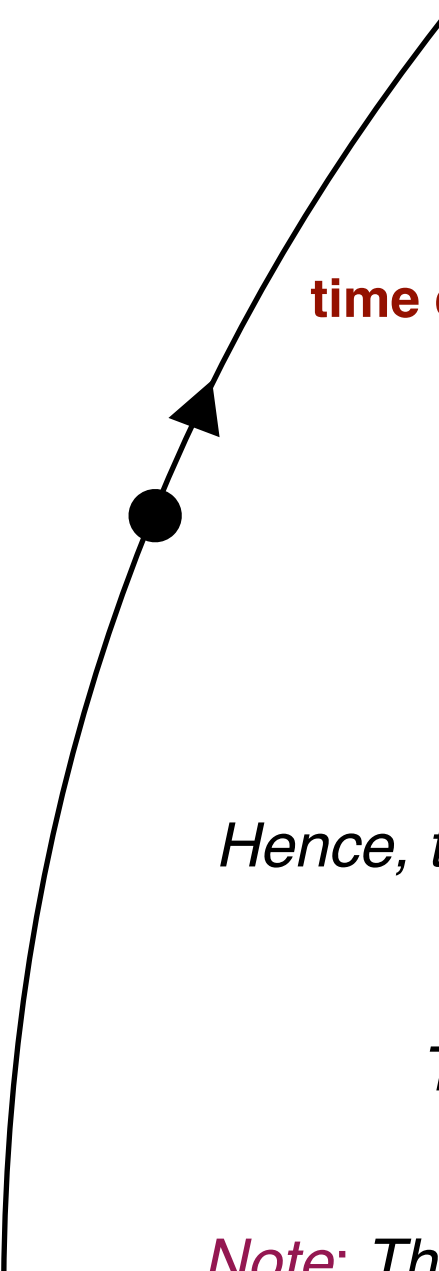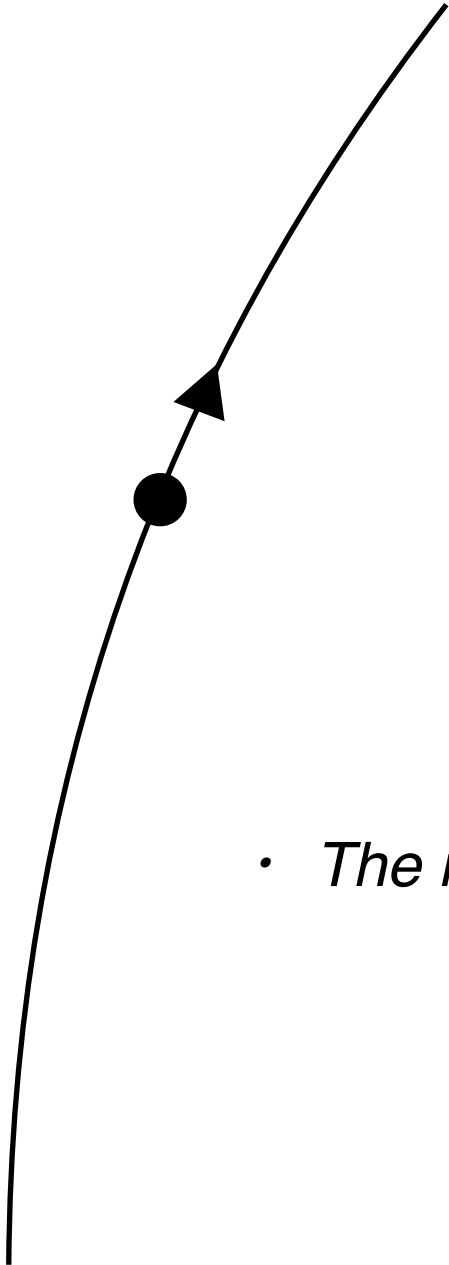
Hence, the Schrodinger equation can be viewed as an operator version of the defining relation for energy in classical mechanics.

This, however, should NOT be taken as a derivation of the SE.

Note: The quantity $H(\mathbf{r}, \boldsymbol{p})$ is known as the Hamiltonian in Classical Mechanics.
It's specific value $H(\mathbf{r}, \boldsymbol{p}) = E$ is what we call Energy.

For the purpose of this course, we shall only be interested in *states* which have *definite energy* in presence of a *time-independent potential*

$$H(\mathbf{r}, \boldsymbol{p}) = E$$

These are described by wave function of the form

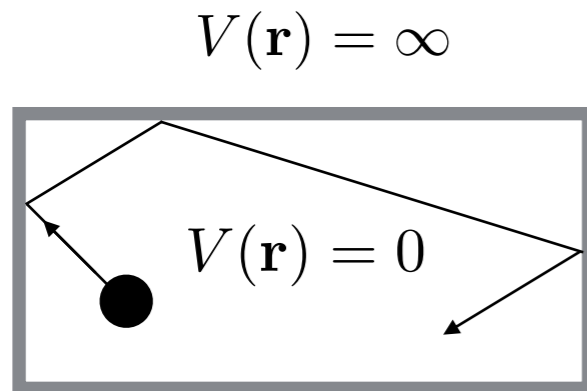$$\psi(\mathbf{r}, t) = u(\boldsymbol{r}) e^{-\frac{iEt}{\hbar}}$$

- *The resultant Schrodinger equation is known as the time-independent SE*

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] u(\mathbf{r}) = E u(\mathbf{r})$$

- *It describes states of a system having a definite energy E*

- *Such states are known as stationary states*

Example 1
A free particle in a one dimensional box

$V(\mathbf{r}) = \infty$

$V(\mathbf{r}) = 0$

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] u(x) = E u(x)$$

zero

$$\frac{d^2 u(x)}{dx^2} = -\left(\frac{2mE}{\hbar^2} \right) u(x)$$

Discuss solutions of this equation
and
discrete nature of possible energies *E*

Example 2
Lowest energy state of a Harmonic Oscillator

$$V(x) = \frac{1}{2}kx^2$$

$$x = 0$$
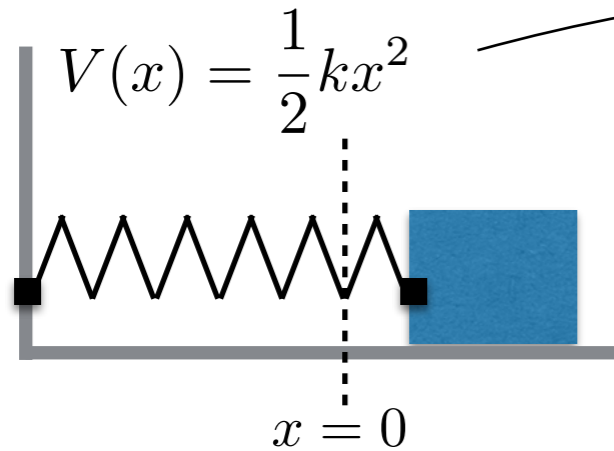
$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \right] u(x) = E u(x)$$

$$\frac{d^2 u(x)}{dx^2} = -\left[\frac{2m}{\hbar^2}\left(E - V(x) \right) \right] u(x)$$

We only mention lowest energy solution of this equation and the corresponding value of *E*

Example 2
Lowest energy state of a Harmonic Oscillator

$V(x) = \frac{1}{2}kx^2$

$x = 0$
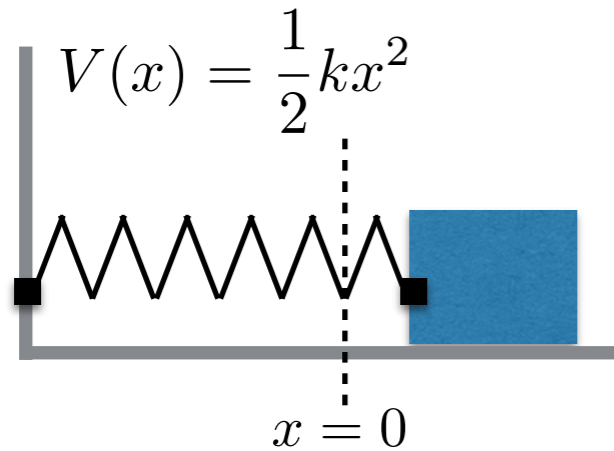
$$\frac{d^2 u(x)}{dx^2} = -\left[\frac{2m}{\hbar^2}\left(E - V(x)\right)\right] u(x)$$

$$u_0(x) = (\alpha/\pi)^{1/4}\, e^{-\alpha x^2/2}$$

$$\alpha = m\omega/\hbar$$

$$\omega = \sqrt{k/m}$$

$$E = E_0 = \frac{1}{2}\hbar\omega$$

This is the so-called ground state of a quantum harmonic oscillator

Example 2
Lowest energy state of a Harmonic Oscillator

$$V(x) = \frac{1}{2}kx^2$$

$$x = 0$$

$$\frac{d^2 u(x)}{dx^2} = -\left[\frac{2m}{\hbar^2}\left(E - V(x)\right)\right]u(x)$$

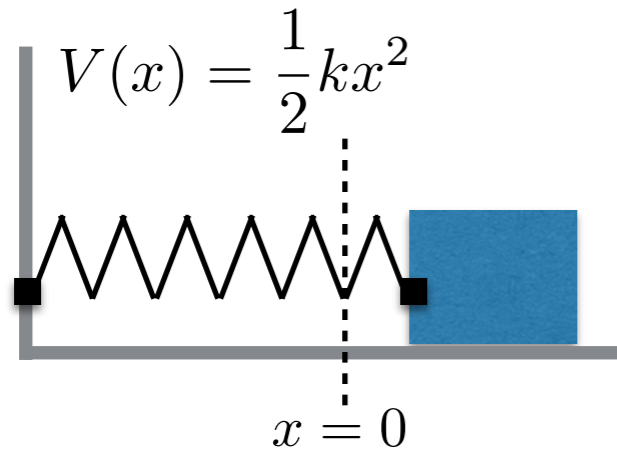$$u_0(x) = (\alpha/\pi)^{1/4}\, e^{-\alpha x^2/2}$$

$$\alpha = m\omega/\hbar$$

$$\omega = \sqrt{k/m}$$
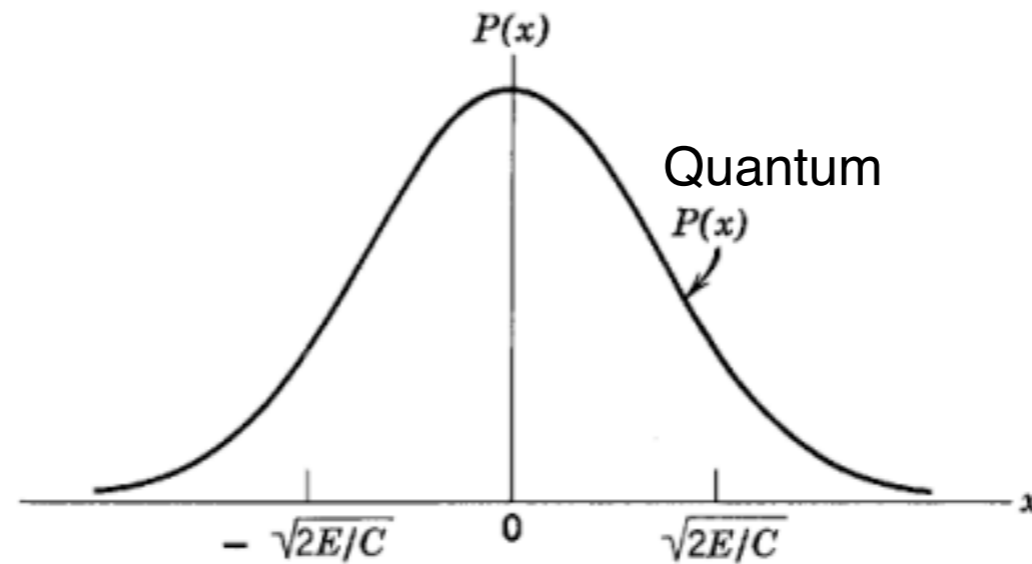
$$E = E_0 = \frac{1}{2}\hbar\omega$$

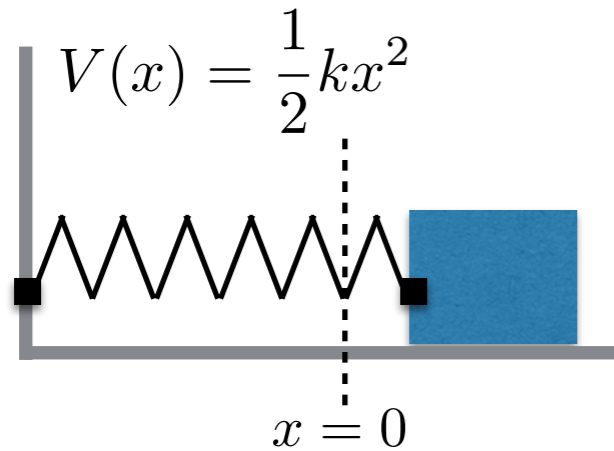**Classical result:** $\quad E = \frac{p^2}{2m} + \frac{1}{2}kx^2 \quad \Rightarrow \quad E_0 = 0$

Here, the lowest energy is zero, which happens for p = 0 = x. In Quantum Mechanics, such a state can not exist!
This is an illustration of the *Uncertainty Principle.*

Example 2
Lowest energy state of a Harmonic Oscillator

$$V(x) = \frac{1}{2}kx^2$$

$x = 0$

$P(x)$

Quantum

$$P(x) = u_0(x)^2$$

$P(x)$

$-\sqrt{2E/C}$ 0 $\sqrt{2E/C}$ x

$P(x)$

$P(x)$ Classical

Classically, the probability for finding the oscillator at a given x is maximum at the turning points, since it spends the most time there.

Quantum mechanically, this probability is maximum at x=0, where the wave function is maximum
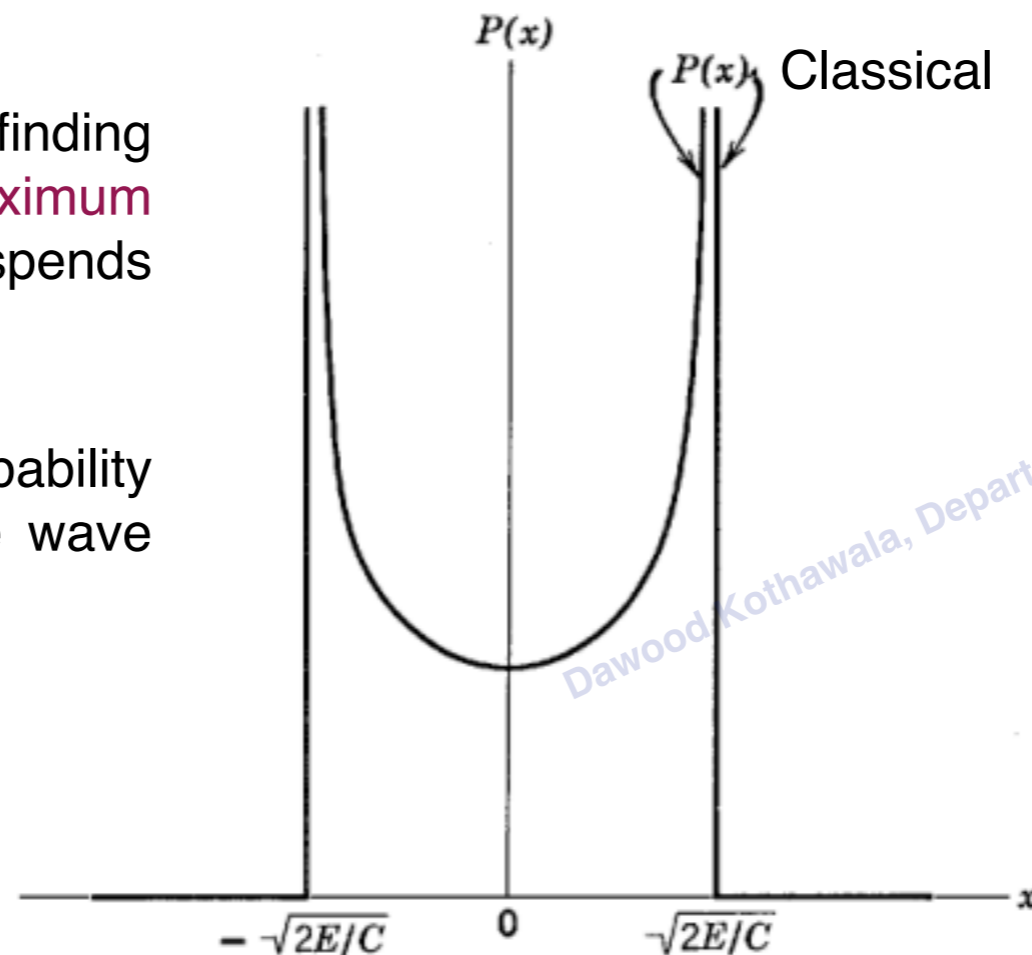
$$P(x) \propto \frac{1}{v(x)}$$

$-\sqrt{2E/C}$ 0 $\sqrt{2E/C}$ x

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Energy Quantization

$$n \in \mathbb{Z}$$

Free particle in a 1D box

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

$$n = \pm 1, \pm 2, \dots$$

Harmonic Oscillator

$$E_n = \left(n + \frac{1}{2} \right) \hbar \omega$$

$$n = 0, 1, \dots$$

Hydrogen atom

$$E_n \approx \frac{(-13.6 \text{eV})}{n^2}$$

$$n = 1, 2, \dots$$

EP2210: Principles of Quantum Mechanics

PH3520: Quantum Physics
PH5825: Quantum Physics