Pázmány Péter Catholic University
Faculty of Information Technology and Bionics

"Fides et Ratio"

Physics of Information Technology II
Physics of Molecular Bionics II
2014 Autumn

Physics of Information Technology I.
Physics of Molecular Bionics I.
MEMO in English
3. Quantum Mechanics

Az Információtechnika Fizikai Alapjai I.
A Molekuláris Bionika Fizikai Alapjai I.
Emlékeztető angol nyelven

1. rész Klasszikus Mechanika és
2. Elektrodinamika (Elméleti Villamosságtan)

Physics of Information Technology I.
Physics of Molecular Bionics I.
MEMO in English

1. Classical Mechanics
2. Classical Electrodynamics)

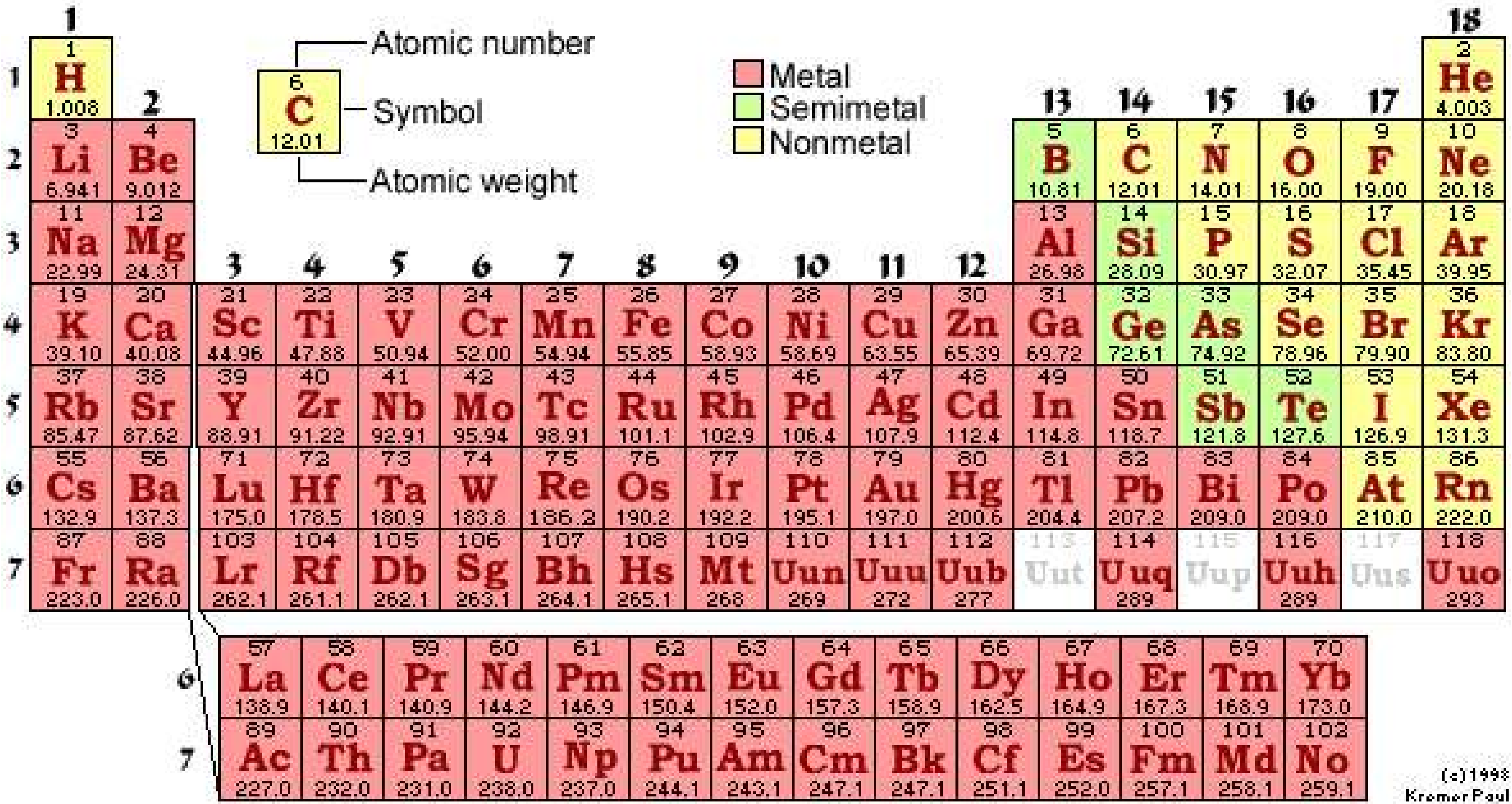
Az Információtechnika Fizikai Alapjai I.
A Molekuláris Bionika Fizikai Alapjai I.
Emlékeztető Angol nyelven
3. Kvantummechnaika

Physics of Information Technology I.
Physics of Molecular Bionics I.
MEMO in English
3. Quantum Mechanics

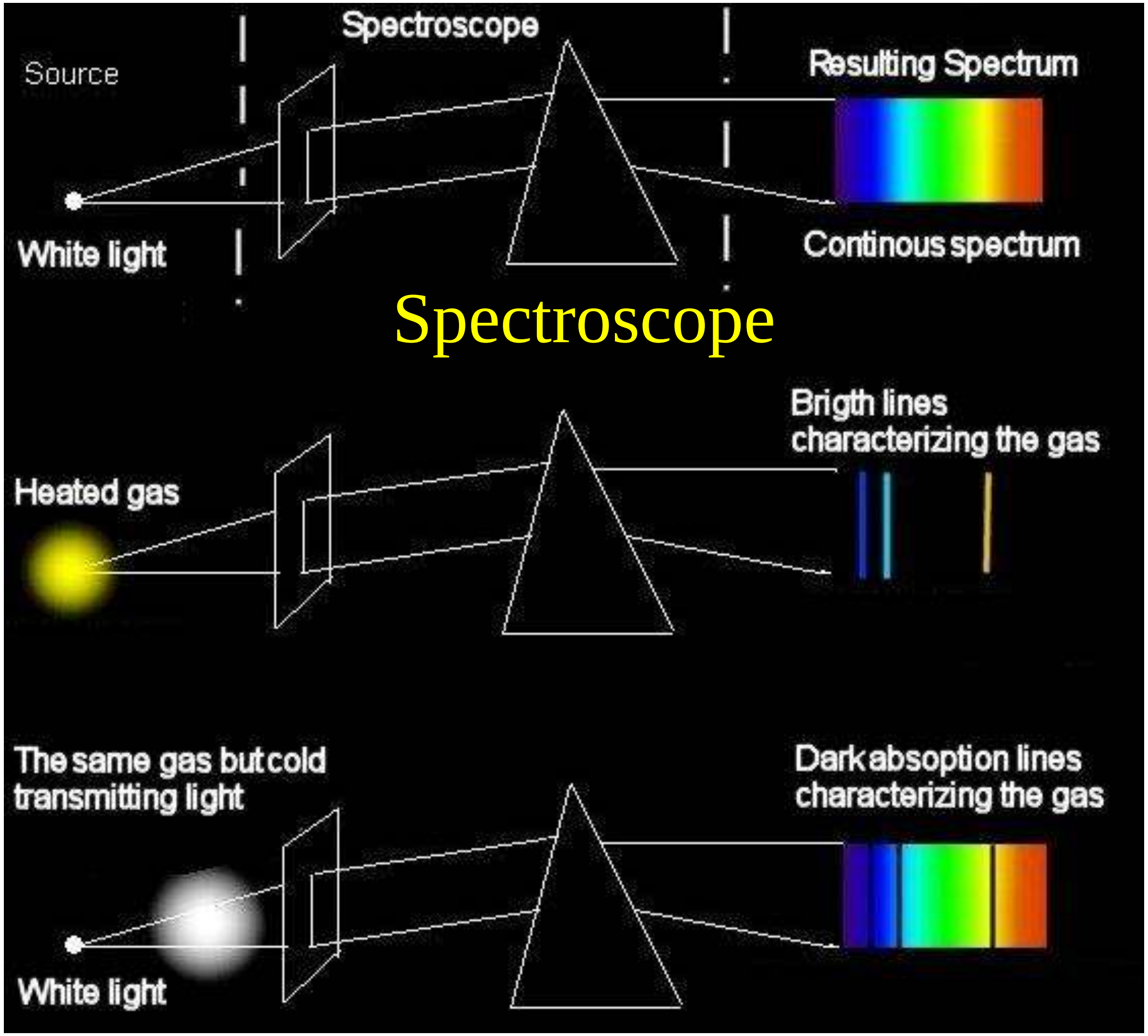
World View at the end of 19th Century

Our experiences are in SPACE and TIME (our "Theatre")

BODIES are composed of neutral "point-like" ATOMS (of mass *m*), and are moving because FORCES act on them



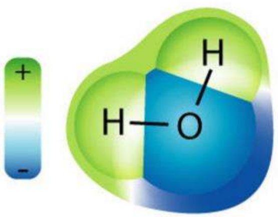
Interaction of LIGHT and BODIES
(Ultraviolet, Visible and Infrared Spectroscopy)



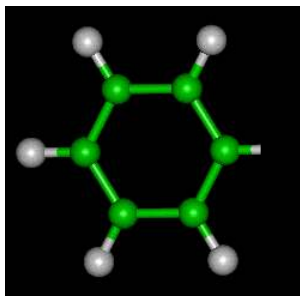
“Self-Assembly” of ATOMS

Self-assembly is a type of process in which a disordered system of pre-existing components forms an organized structure or pattern as a consequence of specific, local interactions among the components themselves, without external direction.

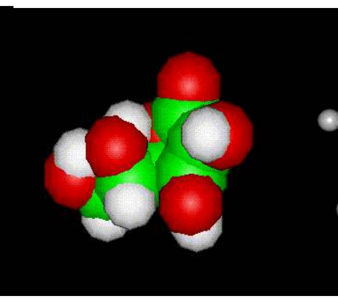
The Water Molecule



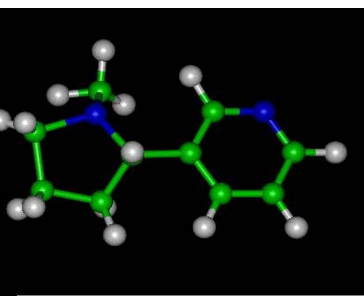
Benzene



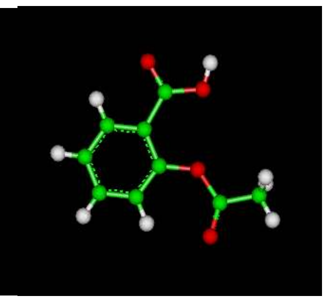
Vitamin C



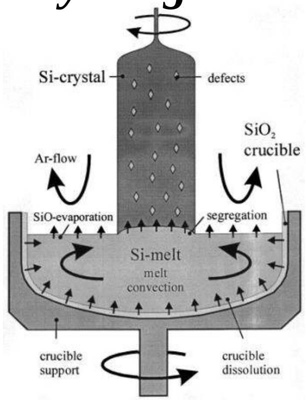
Nicotine

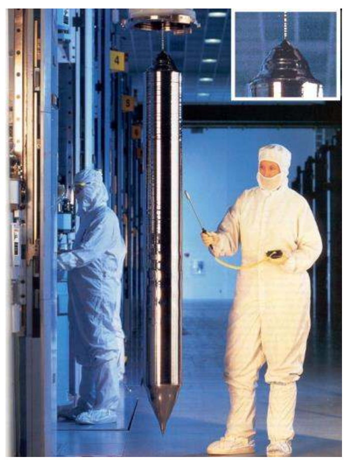


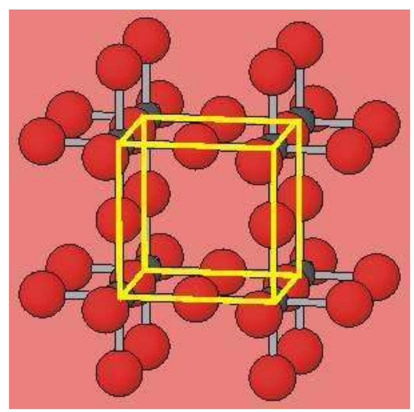
Aspirin

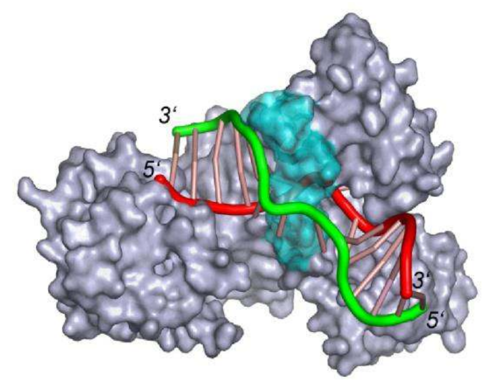


Crystal growth





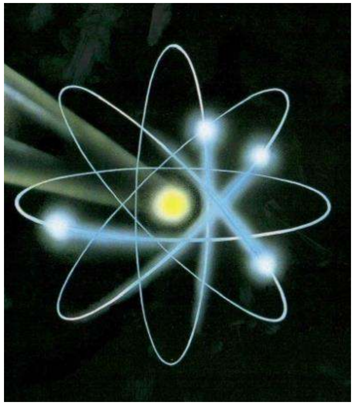




WHAT DO WE KNOW ABOUT THE H ATOM?

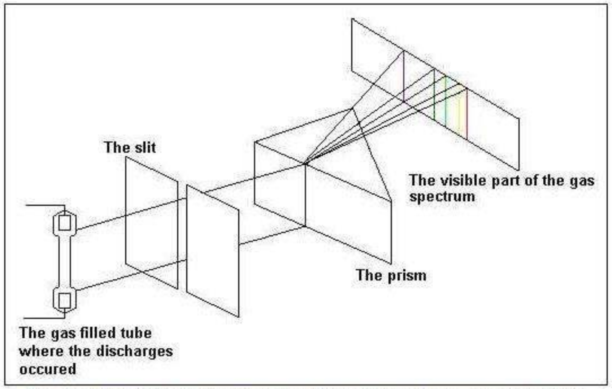
Why not nuclear planetary model? Because troubles:

1. The orbiting electron as a charge should radiate

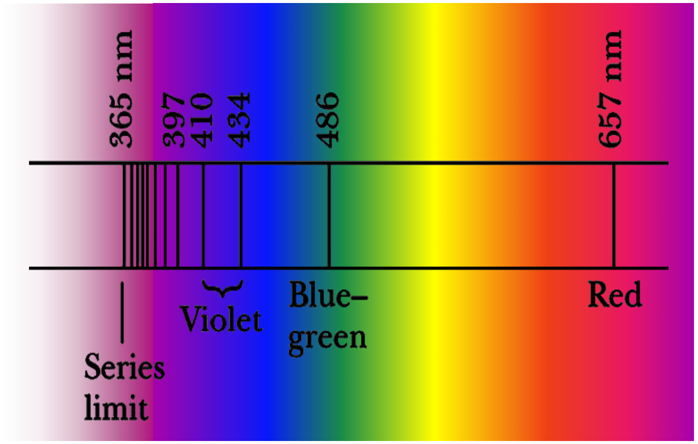


2. If the electron looses energy it should collapse into the nucleus

3. Getting continuously closer to the nucleus, the frequency of radiation should change continuously.



The discharges in the low pressure gas filled tube are the sources of the light which undergo refraction on the prism. We see the line spectrum of the gas.



Radiation spectrum is discrete;

There is no radiation in stationary states.

What do we know about the photon?

The parameters of the photon as a wave $(\omega, \vec{\mathbf{k}})$

The parameters of the photon as a particle $(E, \vec{\mathbf{p}})$

For particles during collision the conservation of energy and momentum holds.

Waves interfere (Constructive , destructive).

WAVE AND PARTICLE NATURES ARE INTERRELATED

$$E = h\nu = \frac{h}{2\pi}\omega = \hbar\omega \qquad \vec{\mathbf{p}} = \frac{h}{\lambda}\vec{\mathbf{n}} = \frac{h}{2\pi}\vec{\mathbf{k}} = \hbar \cdot \vec{\mathbf{k}}$$

$$E = \hbar\omega \qquad \vec{\mathbf{p}} = \hbar \cdot \vec{\mathbf{k}}$$

$$h = 6.625 \cdot 10^{-34}\ \mathrm{Ws}^2$$

$$\hbar = h / 2\pi = 1.05 \cdot 10^{-34}\ \mathrm{Ws}^2$$

Photon's Wave – Particle Duality

$$\omega, \mathbf{k} \qquad E, \mathbf{p}$$

$$E = \hbar\omega = h\nu; \qquad \vec{\mathbf{p}} = \frac{h}{\lambda}\vec{\mathbf{n}} = \frac{h}{2\pi}\vec{\mathbf{k}} = \hbar \cdot \vec{\mathbf{k}}$$

PHOTON IS WAV-e-part-ICLE= „WAVICLE”

de Broglie:

ELECTRON IS A „WAVICLE” ALSO

Electron’s Particle - Wave Duality

The parameters of an electron as a particle $(E, \vec{\mathbf{p}})$

The parameters of an electron as a wave $(\omega, \vec{\mathbf{k}})$

WAVE AND PARTICLE NATURES ARE INTERRELATED

$$E = h\nu = \frac{h}{2\pi}\omega = \hbar\omega \qquad \vec{\mathbf{p}} = \frac{h}{\lambda}\vec{\mathbf{n}} = \frac{h}{2\pi}\vec{\mathbf{k}} = \hbar \cdot \vec{\mathbf{k}}$$

$$E = \hbar\omega \qquad \vec{\mathbf{p}} = \hbar \cdot \vec{\mathbf{k}}$$

$$h = 6.625 \cdot 10^{-34} \text{ Ws}^2$$

$$\hbar = h / 2\pi = 1.05 \cdot 10^{-34} \text{ Ws}^2$$

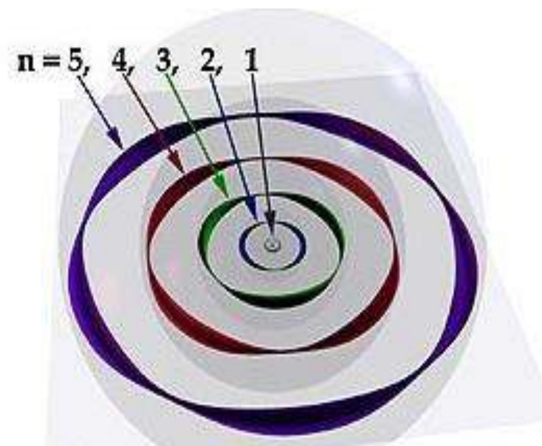
Electrons are also 'wavicles' : the group velocity of the 'wave' is equal to the velocity of the particle,

$$\lambda = \frac{\mathrm{h}}{p} \quad \rightarrow p = m \cdot v = \hbar \cdot k = \frac{\mathrm{h}}{2\pi}\frac{2\pi}{\lambda}$$

De Broglie resolved the mystery of the Bohr's model

$$m v_n r_n = n\frac{\mathrm{h}}{2\pi}, \qquad \text{where} \qquad n = 1, 2, \ldots$$

$$\lambda = \frac{\mathrm{h}}{p} = \frac{h}{m v_n} \Rightarrow \frac{2\pi\, r_n}{n}$$



PHOTOMULTIPLIER - (Bay Zoltán)

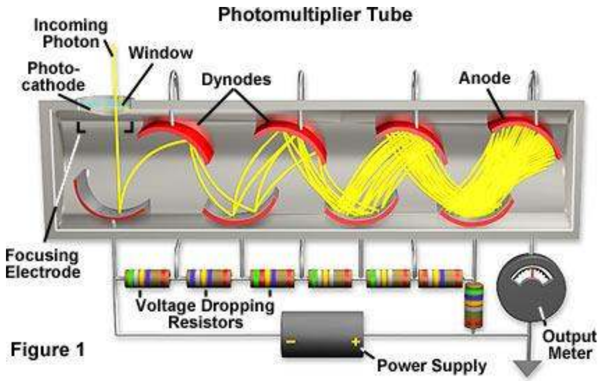
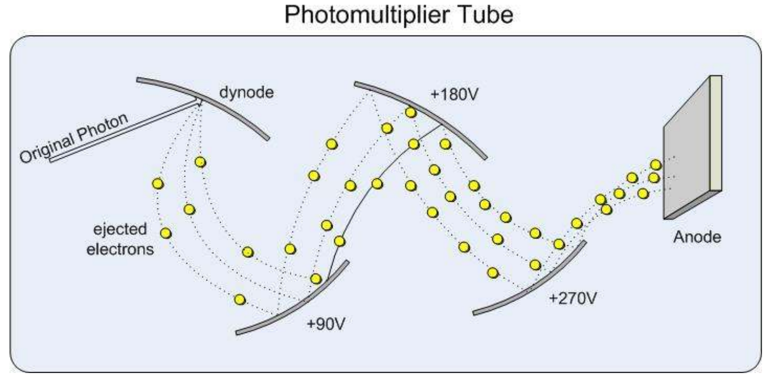
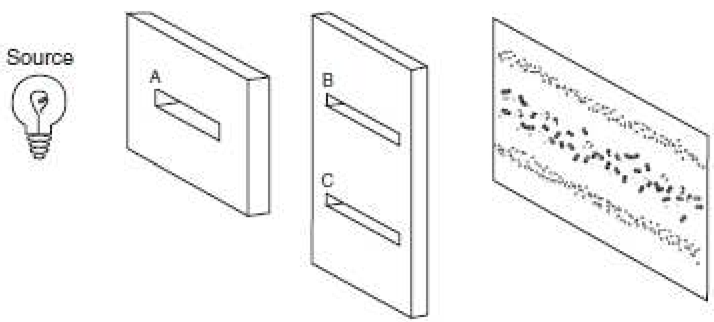


Figure 1

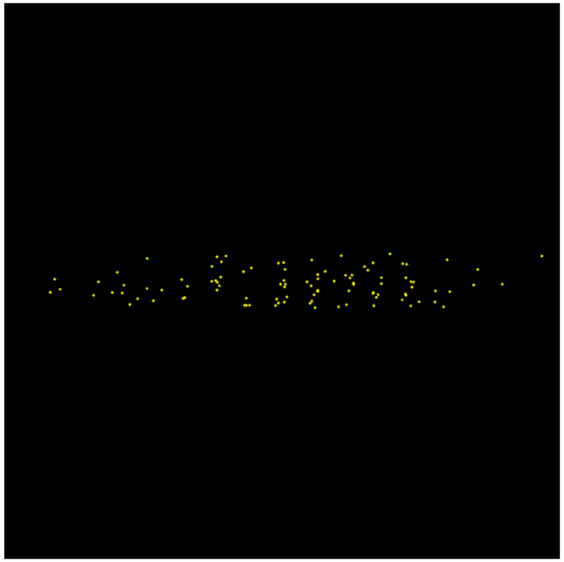


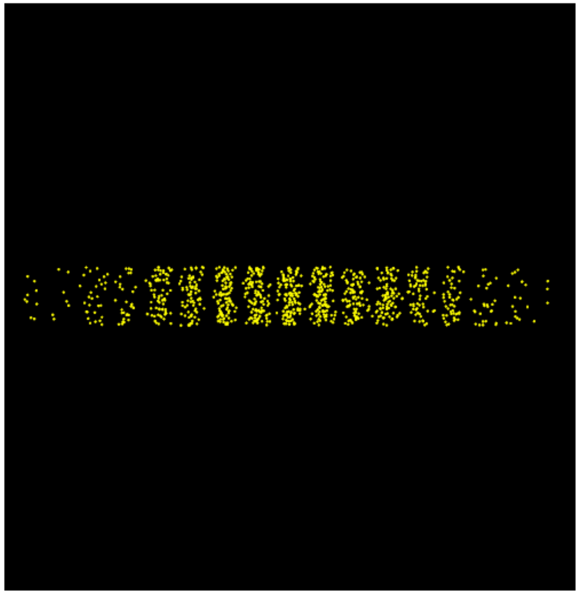
TWO-SLIT EXPERIMENT (PHOTONS)

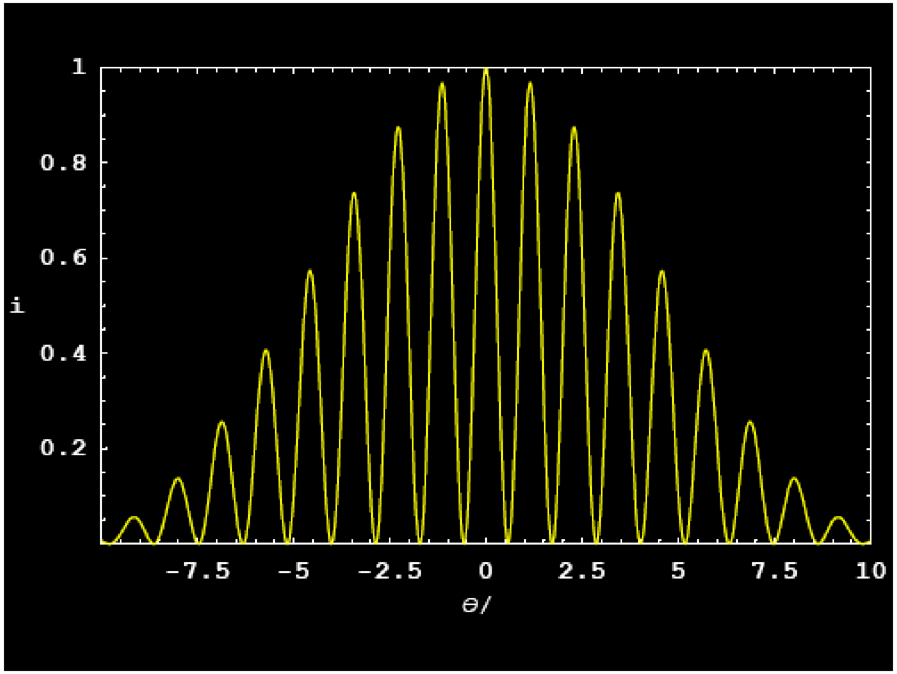


Papers with pure silver bromide emulsions are sensitive and produce neutral black image tones.

Silver bromide (AgBr)

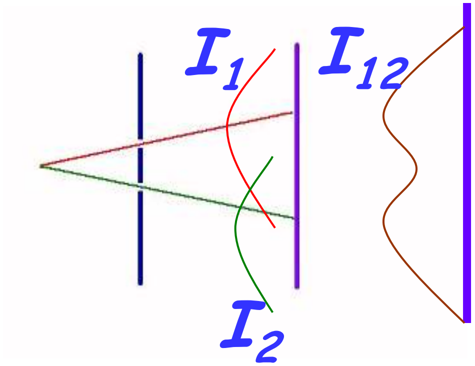






1
0.8
0.6
0.4
0.2
i
-7.5
-5
-2.5
0
2.5
5
7.5
10
θ/

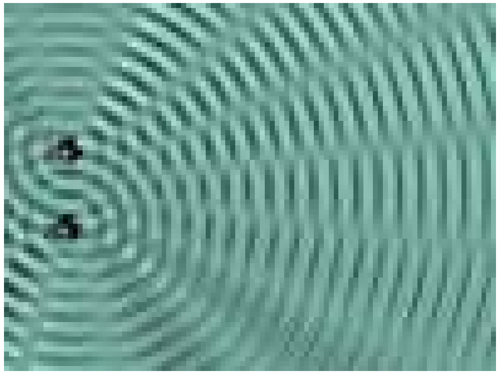
Let us try the two-slit experiment for electrons ?

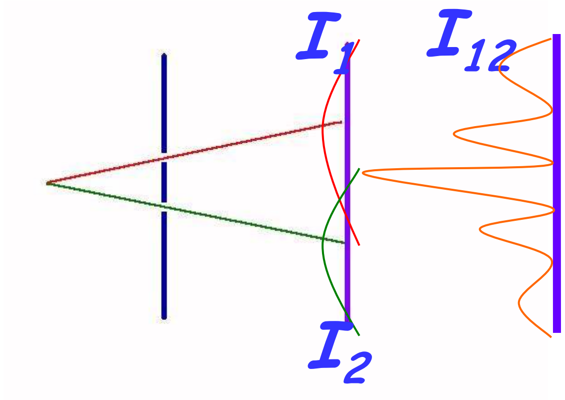


In case of particles (e.g. billiard balls)

$$I_1 + I_2 = I_{12}$$

In case of waves (e.g. water waves)

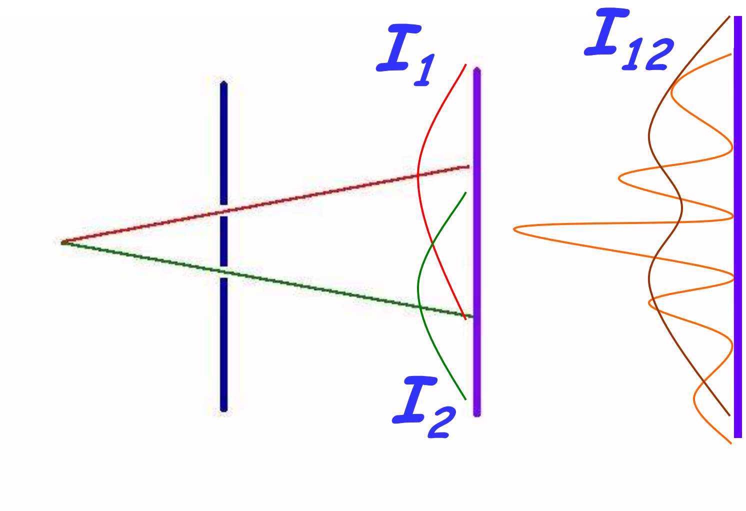




$$I_1 + I_2 \neq I_{12}$$

Interference!

What do we see in case of electrons?



Are electrons like bullets?

$$I_1 + I_2 = ?\, I_{12}$$

$$I_1 + I_2 \neq I_{12}$$

No! We see INTERFERENCE ?!

$$I_1 = |\psi_1|^2 ; I_2 = |\psi_2|^2 ; I_{12} = |\psi_{12}|^2$$

$$\psi_1 + \psi_2 = \psi_{12}$$

On Mondays, Wednesdays and Fridays, it is a PARTICLE!
On, Tuesdays, Thursdays and Saturdays it is a WAVE!

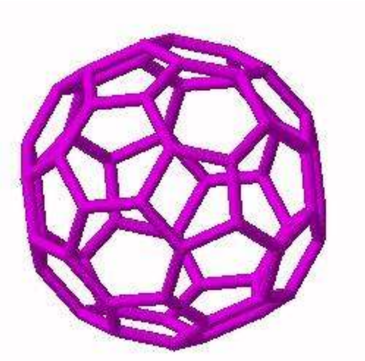
Oh LORD, please, is it a PARTICLE or a WAVE!!???

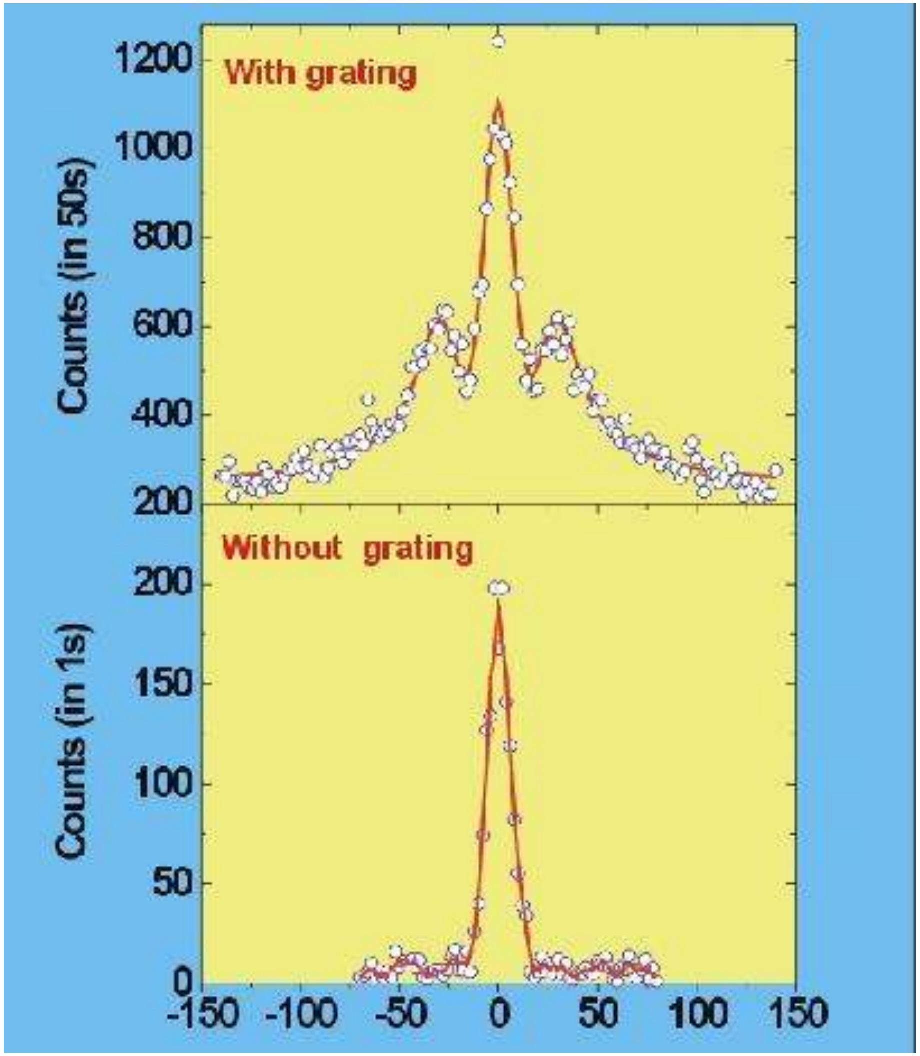
On Sundays

It is both! It has a DUAL NATURE

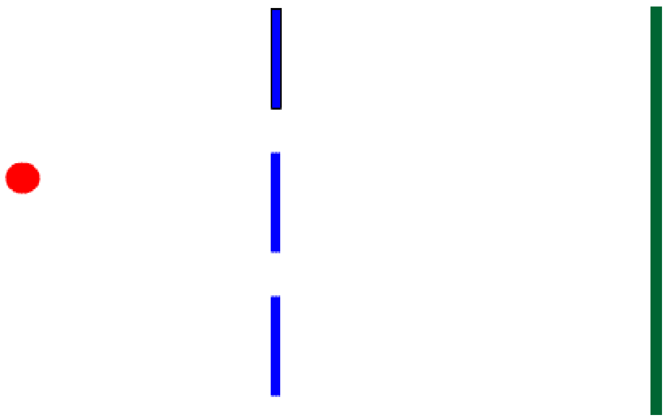
Not only electrons and photons, but EVERYTHING has this dual nature! Experimentally shown for protons, neutrons, He atoms, even C_{60}!

C60





Prof. A. Zeilinger
http://www.quantum.univie.ac.at/zeilinger/

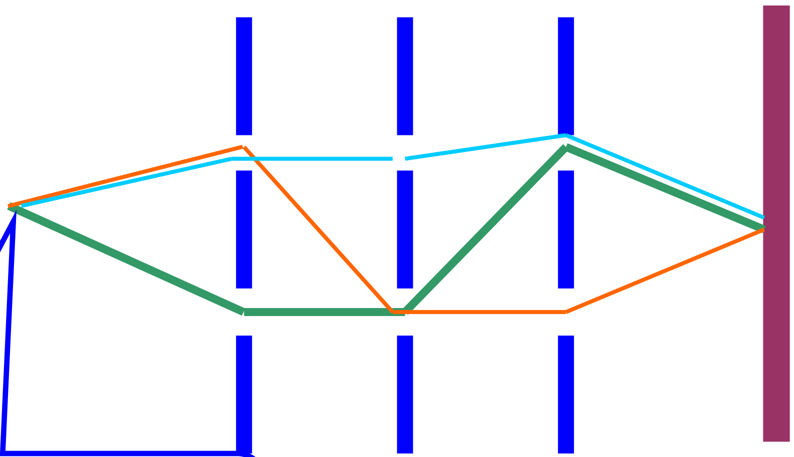


Does it go through both the slits?

How does an electron move (propagate)?

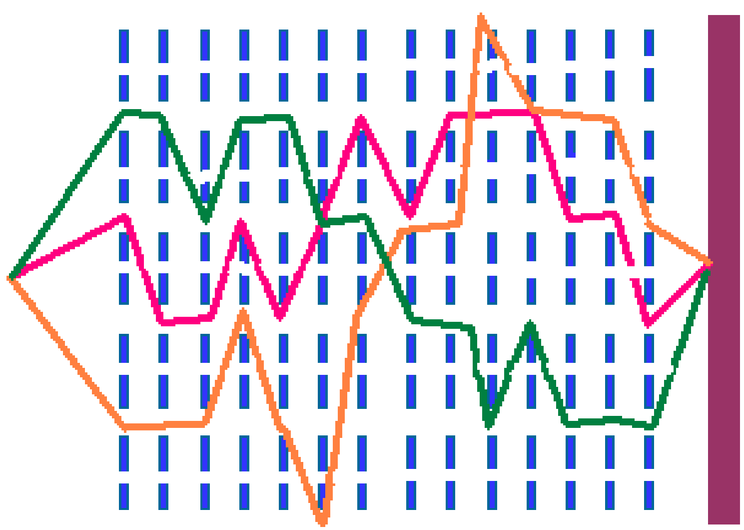
Through all possible paths!

He is crazy!



Source of particles

More slits



Even more Complex setup

SCHRÖDINGER's Wave Mechanics, 1926

Assumptions

1. Planck and de Broglie $\lambda = \frac{\mathrm{h}}{p}, \qquad \nu = \frac{E}{\mathrm{h}}$

2. Energy $E = \frac{p^2}{2m} + E_{\mathrm{pot}}$

3. Linearity in the wave function (interference)

$$\psi\left(x, t\right) \qquad P(x,t) = \left|\psi(x,t)\right|^2$$

$$-\frac{\hbar}{\mathrm{j}}\frac{\partial\psi\left(x,t\right)}{\partial t} = \mathbf{H}\psi\left(x,t\right) \qquad \mathbf{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$$

Schrödinger equation for a single electron in one spatial dimension

Hamilton operator

$$\mathrm{j}\hbar \frac{\partial}{\partial \mathrm{t}} \psi\left(x, t\right) = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_{\mathrm{pot}}\left(x\right) \right) \psi\left(x, t\right) \qquad \forall x, \forall t$$

Single particle in three dimensions

$$\frac{\partial^2 \psi(x,t)}{\partial x^2} \Rightarrow \frac{\partial^2 \psi(x,y,z,t)}{\partial x^2} + \frac{\partial^2 \psi(x,y,z,t)}{\partial y^2} + \frac{\partial^2 \psi(x,y,z,t)}{\partial z^2}$$

$$\equiv \Delta\psi(x,y,z,t) \equiv \Delta\psi(\mathbf{r},t)$$

$$\mathrm{j}\hbar \frac{\partial \psi\left(\mathbf{r}, t\right)}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi\left(\mathbf{r}, t\right) + V_{\mathrm{pot}}\left(\mathbf{r}\right) \psi\left(\mathbf{r}, t\right) = \mathbf{H} \psi\left(\mathbf{r}, t\right)$$

The Postulates of Schrödinger's Quantum Mechanics

Postulate 1. (P.1) *Information we can know about a state*

The state of a system is fully described by its state-function (wave-function) $\psi(q_1, q_2, ..., q_f, t)$, which is bounded, single-valued, continuous, and continuously differentiable function of the configuration-space-coordinates $(q_1, q_2, ..., q_f)$ and of time t .

Postulate 2. (P.2) *Interpretation of the wave-function*

The probability that the system in state ψ can be found in the volume-element $\mathrm{d}V$ of the configuration space is $\psi\psi^*\mathrm{d}V$.
From this it follows that

$$\int_V \psi\psi^* \, \mathrm{d}V = 1$$

i.e. ψ is square-integrable.

Postulate 3. (P.3) O*bservables*

There is a linear operator L assigned to every observable (measurable dynamical variable) *L.*

If we perform a "strong" measurements on the system then the observable's values of *L* are the λ eigen-values of operator L

$$\mathbf{L}\psi=\lambda\psi.$$

$$\mathbf{r} \Rightarrow \mathbf{r}\cdot$$

The rules of the operator assignment are as follows:

a) The operators of the space coordinates are multiplication by the coordinate : $\mathbf{q}_i \quad \longrightarrow \quad q_i;$

b) The operator assigned to the momentum: $\mathbf{p} \rightarrow -\mathrm{j}\hbar\nabla$

c) We assign operators to dynamical variables which are functions of the space coordinates moments by substituting the operators of the space coordinates and moments into the functions:

$$E_{\text{kin}} = \frac{1}{2} m\mathbf{v}^2 = \frac{1}{2m}\mathbf{p}^2 \rightarrow \quad \mathbf{E}_{\text{kin}} = -\frac{\hbar^2}{2m}\nabla^2$$

The operator of the total energy of a particle $\quad E = E_{\text{kin}} + E_{\text{pot}}$

$$\mathbf{H} = -\frac{\hbar^2}{2m}\Delta + E_{\text{pot}}(\mathbf{r})$$

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

where $\nabla^2 = \Delta$, which in Descartes-coordinates:

The operator of a particle’s angular momentum:

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \quad \rightarrow \quad \mathbf{L} = -\mathrm{j}\hbar \mathbf{r} \times \nabla$$

Hamilton operator of a many-body system

$$E = E_{\text{kin}} + E_{\text{pot}} = \sum_{i=1}^{n} \frac{1}{2m_i}\mathbf{p}_i^2 + E_{\text{pot}} \;\; \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_n$$

$$E_0 = 0.5 \;\; E_{n+1} - E_n$$

Postulate 4. (P.4) *The outcome of strong measurements*

If the state of a physical system is ψ, and we observe the dynamic *observable L with operator L, then the expectation value and deviation of L are:*

$$\langle L \rangle = \int_V \psi^* \mathbf{L} \psi \, \mathrm{d}V \qquad \Delta L = \sqrt{\langle L^2 \rangle - \langle L \rangle^2}$$

Postulate 5. (P.5) *Time-evolution of the wave-function*

In a closed system the wave-function evolves in time according to the time-dependent Schrödinger equation:

$$\mathrm{j}\hbar \frac{\partial \psi}{\partial t} = \mathbf{H} \psi$$

(From the initial sate-function ψ_{t_0} we can determine the future of the wave-function ψ_t for $t > t_0$).

$$h = 6.625 \cdot 10^{-34} \ \mathrm{Ws}^2$$

$$\hbar = h / 2\pi = 1.05 \cdot 10^{-34} \ \mathrm{Ws}^2$$

“Bounded” electron

Discrete energy spectrum

$$E_{k1}, E_{k2}, \ldots, E_{kn}, \ldots$$

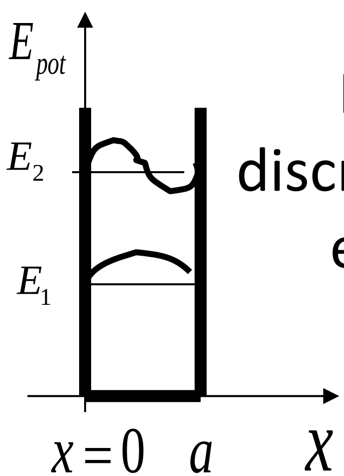
$$\psi(x,t) = \sum_n c_n \psi_n(x)\, e^{-\mathrm{j}\frac{E_n}{\hbar}t}$$

„Free” electron

Continuous energy spectrum

$E(k)$ continuous function

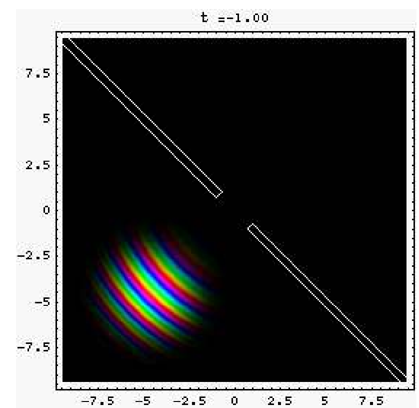
$$\psi(x,t) = \int_{-\infty}^{+\infty} A(k) e^{\mathrm{j}(kx - \frac{E}{\hbar}t)} \mathrm{d}k$$



Electron in discrete stationary eigenstates

Wave pocket

(linear combination of waves with continuous k wave numbers)



Consequences of the Postulates

Frequency, period in time

1. Total energy $E = h \cdot \nu = \hbar \cdot \omega$ $\Rightarrow$ $e^{-j \cdot \omega t} = e^{-j\frac{E}{\hbar}t}$

2. Momentum $\mathbf{p} = \hbar \cdot \overline{\mathbf{k}}$ $p = \hbar \cdot k = \dfrac{h}{\lambda}$

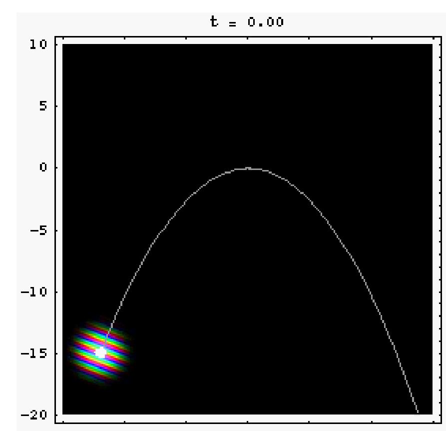
Wavelength, period in space

3. Electrons are either 'bounded' or 'free'

Example1: Bounded in a one-dimensional box

$$E_n = \frac{h^2}{8ma^2} n^2, \quad \psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x \cdot e^{-\mathrm{j}\frac{E_n}{\hbar}t}, \quad n = 1, 2, \ldots$$

Example2: Free electron in vacuum



How does the Expectation Value of Measurements Change in Time?

$$\langle L \rangle = \int_V \psi^* \mathbf{L} \psi \, \mathrm{d}V = \langle \psi | \mathbf{L} | \psi \rangle \qquad \frac{\mathrm{d}\langle L \rangle}{\mathrm{d}t} = \left\langle \frac{\partial \psi}{\partial t} \middle| \mathbf{L} \middle| \psi \right\rangle + \left\langle \psi \middle| \mathbf{L} \middle| \frac{\partial \psi}{\partial t} \right\rangle$$

$$\frac{\partial \psi}{\partial t} = -\frac{\mathrm{j}}{\hbar} \mathbf{H} \psi \rightarrow \frac{\mathrm{d}\langle L \rangle}{\mathrm{d}t} = \frac{\mathrm{j}}{\hbar} \langle \mathbf{H}\psi | \mathbf{L} | \psi \rangle - \frac{\mathrm{j}}{\hbar} \langle \psi | \mathbf{L} | \mathbf{H}\psi \rangle$$

$$\frac{\mathrm{d}\langle L \rangle}{\mathrm{d}t} = \frac{\mathrm{j}}{\hbar} \langle \psi | \mathbf{HL} | \psi \rangle - \frac{\mathrm{j}}{\hbar} \langle \psi | \mathbf{LH}\psi \rangle = \frac{\mathrm{j}}{\hbar} \langle \psi | \mathbf{HL} - \mathbf{LH} | \psi \rangle \qquad \mathbf{HL} - \mathbf{LH} \equiv [\mathbf{H}, \mathbf{L}]$$

„Commutator”

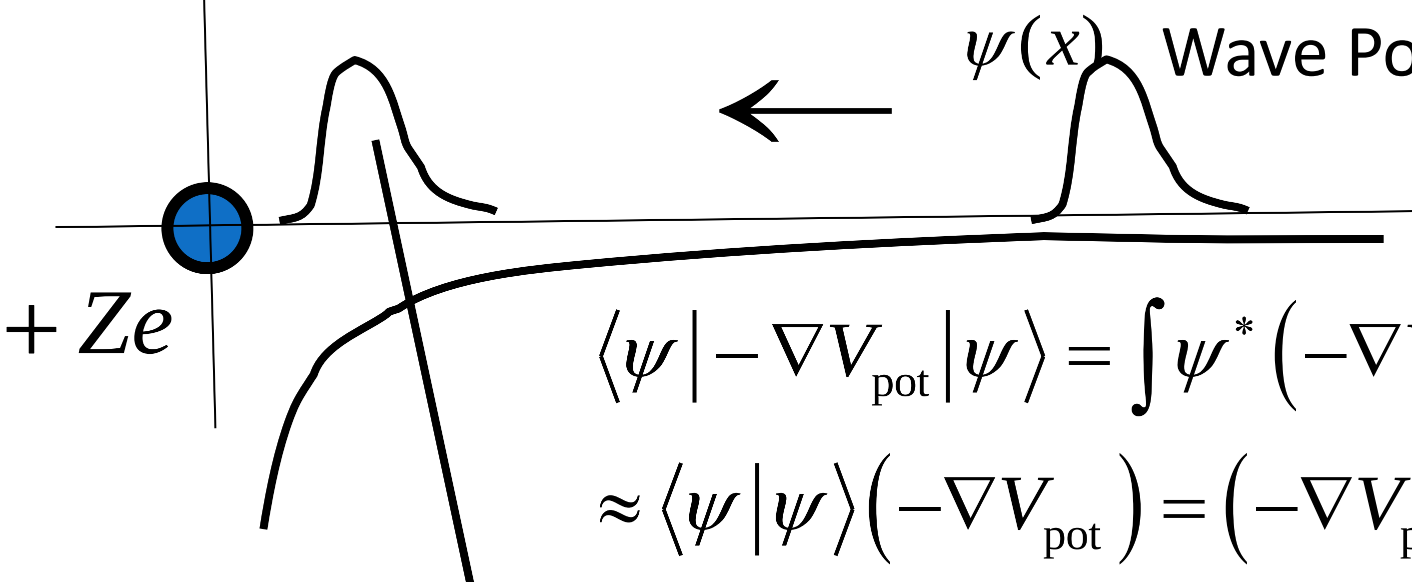
Ehrenfest theorem

$$\frac{\mathrm{d}\langle p \rangle}{\mathrm{d}t} = \frac{\mathrm{d}\langle \psi | \mathbf{P} | \psi \rangle}{\mathrm{d}t} = \langle \psi | -\nabla V_{\mathrm{pot}} | \psi \rangle$$

$$-\nabla V_{\mathrm{pot}} = -\partial V_{\mathrm{pot}} / \partial x = F$$

Electron’s Wave Pocket Flying Toward a Proton

$$\frac{\mathrm{d}\langle p\rangle}{\mathrm{d}t}=\frac{\mathrm{d}\langle\psi|\mathbf{P}|\psi\rangle}{\mathrm{d}t}=\langle\psi|-\nabla V_{\mathrm{pot}}|\psi\rangle \qquad -\nabla V_{\mathrm{pot}}=\partial V_{\mathrm{pot}}/\partial x$$



$$\langle\psi|-\nabla V_{\mathrm{pot}}|\psi\rangle=\int\psi^*\left(-\nabla V_{\mathrm{pot}}\right)\psi\cdot\mathrm{d}r\approx$$

$$\approx\langle\psi|\psi\rangle\left(-\nabla V_{\mathrm{pot}}\right)=\left(-\nabla V_{\mathrm{pot}}\right)$$

The force is not constant even appr. anymore in the wave-pocket

The trajectory of the expectation value is not the classical trajectory anymore

06_03a_Fall.mov

06_04b_ObliqueTrajectory.mov

04_16aSingleSlit.mov

04_18a_TwoSlit.mov

Classical Mechanics | Time t | Quantum Mechanics

Configuration space $q_1, q_2, \ldots, q_i, \ldots q_f$.

Potential energy $E_{\mathrm{pot}} = E_{\mathrm{p}}\left(q_1,\ q_2,\ \ldots,\ q_f\right)$.

Trajectory

$q_1(t), q_2(t), q_3(t), \ldots, q_f(t)$

Kinetic energy

$E_{\mathrm{kin}} = E_{\mathrm{k}}\left(q_1, \ldots, q_f,\ \dot{q}_1, \ldots, \dot{q}_f\right)$.

'Lagrangian' $L = E_{\mathrm{k}} - E_{\mathrm{p}}$.

Generalized momentum $p_i = \dfrac{\partial L}{\partial \dot{q}_i}, i = 1, 2, \ldots, f$.

'Hamiltonian'

$$H(p,q) = \sum_i \dot{q}_i p_i - L$$

Hamilton Equations

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad \dot{q}_i = \frac{\partial H}{\partial p_i}$$

Wave function (Complex)

$$\psi(q_1, q_2, \ldots, q_f, t)$$

Probability $|\psi|^2 = \psi\psi^*$

Total energy E

Hamilton Operator $\mathbf{H}$

Schrödinger Equation

$$\mathrm{j}\hbar \frac{\partial \psi}{\partial t} = \mathbf{H}\psi$$

$$q_1, q_2, ..., q_i, ...q_f.$$

Schrödinger Equation

$$\mathrm{j}\hbar \frac{\partial \psi\left(q_1, ..., q_f, t\right)}{\partial t} = \mathbf{H}\psi\left(q_1, ..., q_f, t\right)$$

$$\psi\left(q_1, ..., q_f, t\right) = \Psi\left(q_1, ..., q_f\right) \cdot \varphi(t)$$

$$\mathbf{H}\Psi = E\Psi \qquad \mathrm{d}\varphi(t)/\mathrm{d}t = -\mathrm{j}\frac{E}{\hbar}\varphi(t)$$

$$E_1, E_2, ..., E_n, ...$$

$$\Psi_1, \Psi_2, ..., \Psi_n, ... \qquad e^{-\mathrm{j}\frac{E_n}{\hbar}t}$$

$$\psi\left(q_1, ..., q_f, t\right) = \sum_n C_n \Psi_n\left(q_1, ..., q_f\right) \cdot e^{-j\frac{E_n}{\hbar}t}$$