GRAN SASSO SCIENCE INSTITUTE
SCHOOL OF ADVANCED STUDIES
Scuola Universitaria Superiore

Quantum Mechanics: a historical introduction

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Physics at the turn of the 19th century

Classical Mechanics tested by new phenomena

At the end of the 19th century **Classical Mechanics** and **Classical Statistical Mechanics** are very well established:

- ⇝ Newton theory
- ⇝ Thermodynamics and kinetic theories
- ⇝ Electromagnetic theory and Maxwell equations
- ⇝ geometrical and physical optics understood in terms of electromagnetic waves

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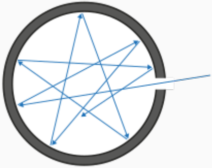
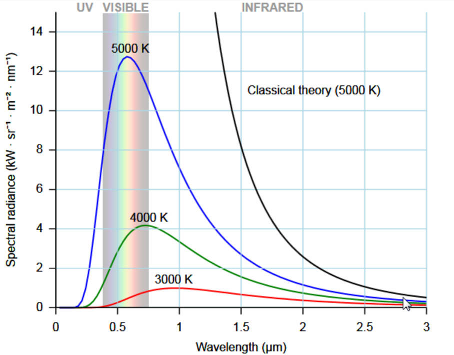
However, Classical Physics is inadequate to describe some phenomena related to **emission and absorption of light**.

The black body radiation

Black body: the incident light is all absorbed, and the equilibrium condition depends only on the temperature T.





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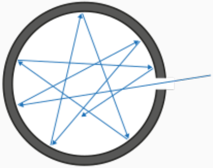

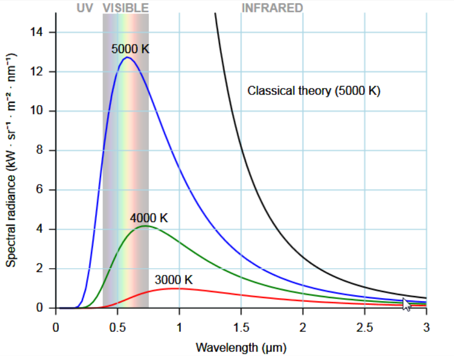

Classical model: the atoms of the walls are described as charged harmonic oscillators in equilibrium with e.m. field.

Electromagnetism and Statistical Mechanics predict that the energy/volume of the radiation satisfies $u(\nu, T) \propto \nu^2 T$.

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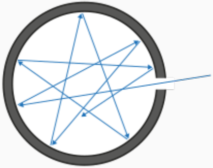

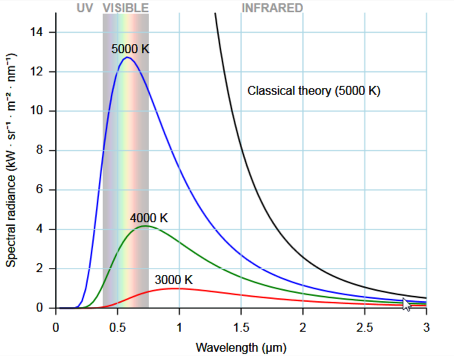

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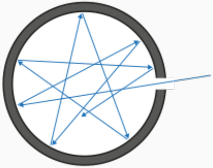

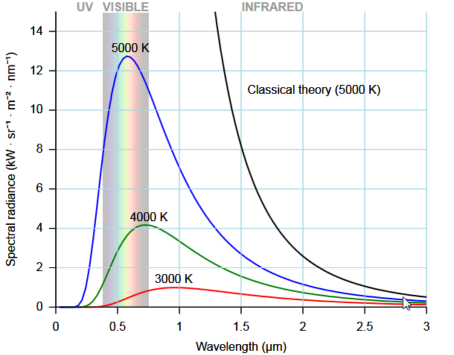

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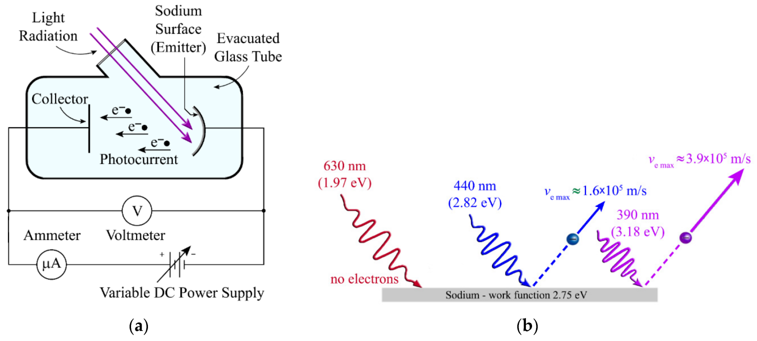
$$h = \text{Planck constant} \sim 10^{-27}\,\text{Joule-seconds}$$

Units: $[h] = \text{Energy} \times \text{Time (Action)}$ and $[\nu] = 1/\text{Time}$.

The surface of a conductor hit by a beam of light emits electrons:



The Photoelectric Effect

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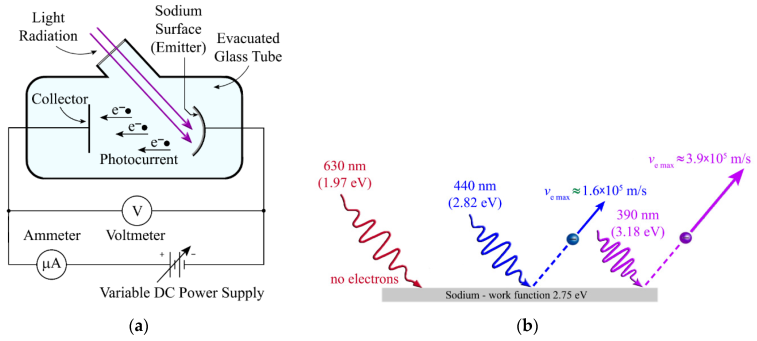

Observations:

i. e^- emitted only if the frequency is larger than a given value;

ii. the kinetic energy of the e^- has a maximum;

iii. number of e^-/second is proportional to the beam intensity.

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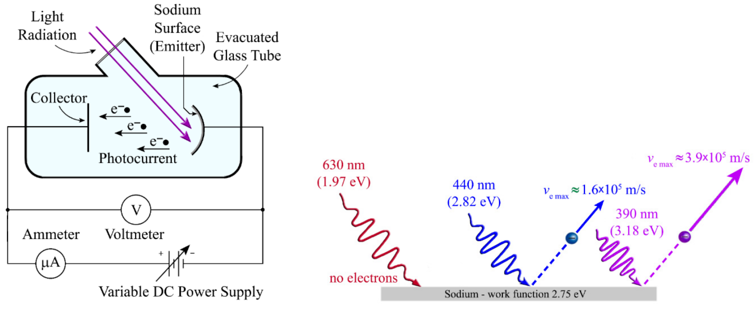

(a) (b)

Einstein (1905): the extraction of an electron results from the interaction between a **single quantum of radiation** and a **single atom of the metal**.

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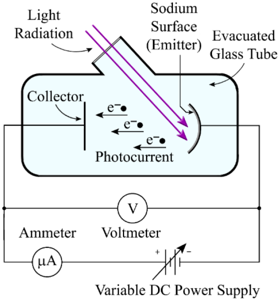
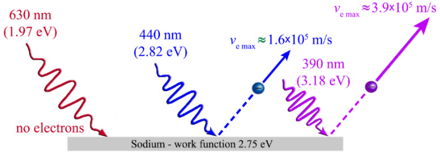


(a)

The light is exchanged in bundles, and **it travels in bundles**.



(b)

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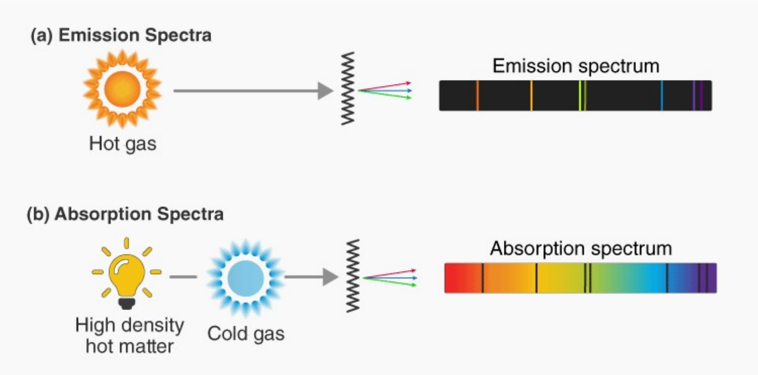
Emission and Absorption Spectra

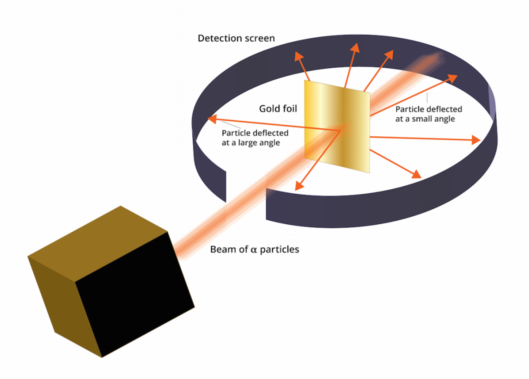


Balmer formula: the frequencies λ_n of the emission and absorption spectra of the hydrogen atom are given by:

$$\frac{1}{\lambda_n} = R\left(\frac{1}{4} - \frac{1}{n^2}\right), \quad n = 3, 4, \ldots$$

Atomic structure of matter

Rutherford (1911): the atom has **lots of free space**. Its mass is concentrated in a tiny nucleus $\sim 10^{-13} cm$, surrounded by electrons moving far apart (atom radious $\sim 10^{-8} cm$).



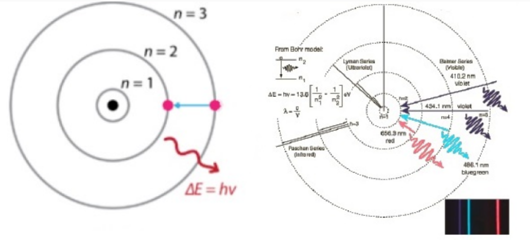
Main problem:

Electric charges in movement radiate according to Maxwell equations; how can the atom be stable?

A new theory

Bohr model-atom (1913)

1. For most of the time no emission;
2. For a very short period of time there is emission of e.m. radiation with frequency $\nu_{ij} = |E_i - E_j|/h$;
3. The electron can have only discrete energies: $E_n = -\frac{1}{2}h\nu_e n$.



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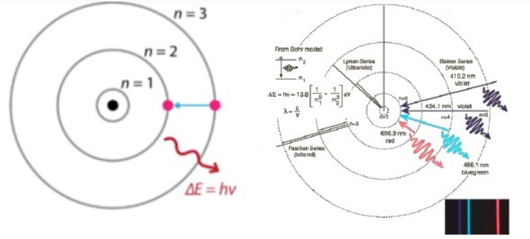

Predictions: energy levels and amplitude of the e$^-$ orbits

$$E_n = -\frac{2\pi^2}{h^2} \frac{e^4 m_e}{n^2}, \qquad a_n = \frac{h^2 n^2}{4\pi^2 e^2 m_e} \qquad n = 1, 2, 3, \ldots$$

A long story made short

1913-24 The old quantum theory (Born, Sommerfeld)

Limitations: only bounded orbits, difficulties with multielectron atoms, lack of internal coherence

1925-26 The new theory

Matrix Mechanics: Heisenberg, Born, Jordan, Dirac

Focus on the observables: e.g. amplitudes and frequencies of the emitted radiation (A_{nm}, ν_{nm})

Wave mechanics: De Broglie, Schrödinger

Focus on the wave behaviour: the electron is described by a scalar function $\psi(x, t)$

A paradigmatic example

The electron two slits experiment

Davisson, Germer (1927): **W** is a source of electrons, **H1** and **H2** holes. On the photographic plate **G** scintillations are observed, which are interpreted as electron impacts on the plate.

Fig. 1. Electron gun.

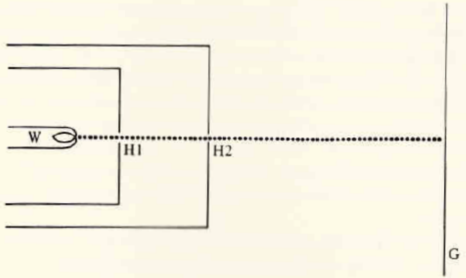

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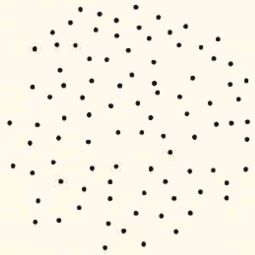
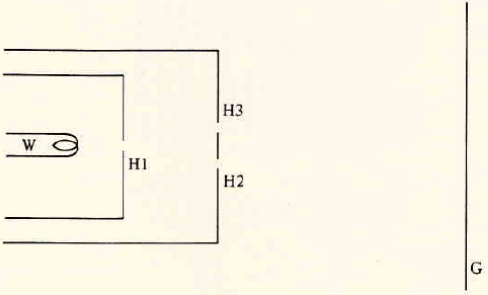
Fig. 2. Pattern built up by many pulses of electron gun of Fig. 1.



A typical output for small linear size of H2. The smaller is H2 the larger is the linear size of the region occupied by the spots.

Let us now perform the experiment using two holes:

Fig. 3. Electron gun with two holes in second screen.



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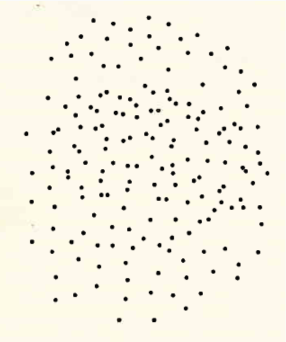

Classical Mechanics
expected pattern

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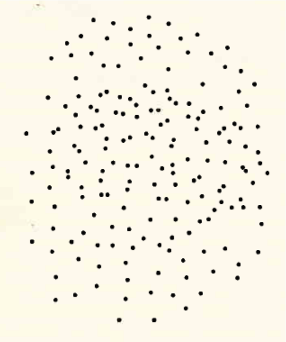

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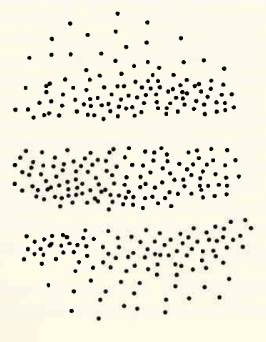
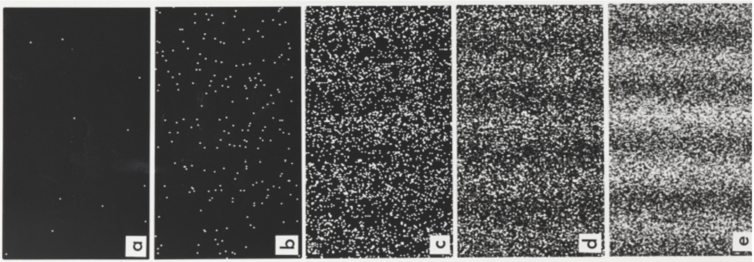


Actual pattern

Dynamics of the spot formation



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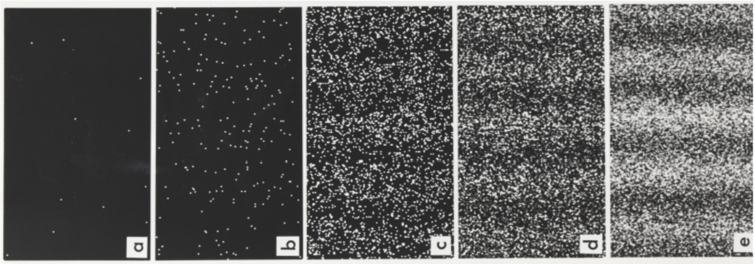
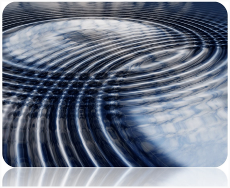
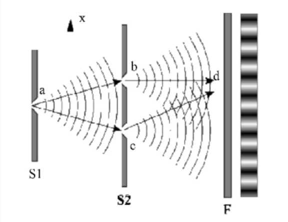
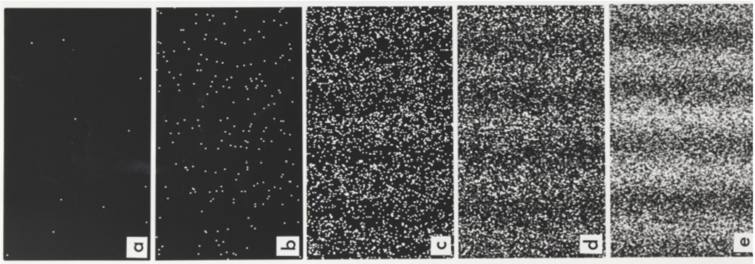


After many identically prepared experiment, the overall scheme of spots looks like the interference pattern in water waves







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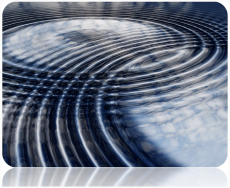

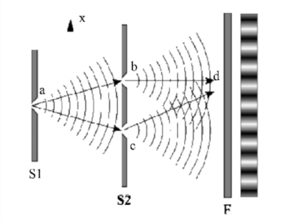

De Broglie '24:
$\lambda_B = h/|p|$

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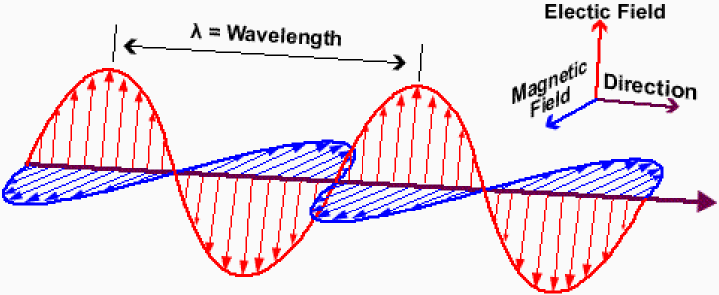
- In spite of an identical initial experimental preparation, impacts are distributed in a macroscopic region of the plate. As a result, only a statistical description of impact positions is possible → ontological probability

- The impact positions statistics differs qualitatively and quantitatively from the one observed when a single hole is open → effect of measurement in Quantum Mechanics

The Schrödinger equation

following the line of thought of Wave Mechanics

The wave equation in optics



Schrödinger equation: derivation by optical analogy

Evolution of the generic component u of the electric field in the scalar optics approximation

$$\Delta u(x,t) - \frac{1}{v_f^2(x)}\,\partial_t^2 u(x,t) = 0\,, \qquad v_f = \lambda\,\nu\,.$$

where $v_f(x) = n(x)/c$ is the phase velocity, $n(x)$ the refraction index of the medium, c the speed of sound.

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The monocromatic component of u satisfies

$$\Delta \tilde{u}(x,\nu) + \frac{4\pi^2\nu^2}{v_f^2(x)}\,\tilde{u}(x,\nu) = 0\,,$$

with $\tilde{u}(x,\nu) = \int dt\, e^{i2\pi\nu t} u(x,t)$.

Schrödinger equation: derivation by optical analogy

Analogy between Geometrical Optics and Classical Mechanics:

the trajectory of a **point particle** with mass m, energy E and subject to a potential $V(x)$

coincides

with the **trajectory of a light** propagating in a medium with phase velocity

$$v_f(x) = \frac{E}{\sqrt{2m\,(E - V(x))}}$$

Schrödinger equation: derivation by optical analogy

Wave Optics (Maxwell)

$\Delta \tilde{u}(x,\nu) + 4\pi^2 \frac{\nu^2}{v_f^2(x)} \tilde{u}(x,\nu) = 0$

$\downarrow \lambda \to 0$

Geometrical Optics (Fermat)

$v_f(x) = c/n(x)$

Wave Mechanics (Schrödinger)

?

$\downarrow h \to 0$

Classical Mechanics (Newton)

$m, E, V(x)$

Geometrical Optics $\longleftrightarrow$ Classical Mechanics: $v_f(x) = \frac{E}{\sqrt{2m\,(E - V(x))}}$

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Idea: we associate to the microscopic particle a wave with

phase velocity: $v_f(x) = \frac{E}{\sqrt{2m(E - V(x))}}$ (optical analogy)

frequence: $\nu = E/h$ (Planck-Einstein).

In particular: $\lambda(x) = \frac{v_f(x)}{\nu} = \frac{h}{\sqrt{2m(E-V(x))}} = \frac{h}{|p|}$ (De Broglie).

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Wave Mechanics (Schrödinger)

$$\Delta \tilde{\psi}(x,\nu) + 4\pi^2 \frac{2m(E-V(x))}{h^2} \tilde{\psi}(x,\nu) = 0$$

$\lambda \to 0$ (Wave Optics → Geometrical Optics)

$h \to 0$ (Wave Mechanics → Classical Mechanics)

Geometrical Optics (Fermat) ⟷ Classical Mechanics (Newton)

$v_f(x) = c/n(x)$ $\quad v_f(x) = \frac{E}{\sqrt{2m\,(E-V(x))}}$ $\quad m, E, V(x)$

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The stationary Schrödinger equation:

By analogy we assumed that $\tilde{\psi}(x, \nu) = \int dt\, e^{2\pi i \nu t} \psi(x, t)$ satisfies

$$\Delta \tilde{\psi}(x, \nu) + 4\pi^2 \, \frac{2m(E - V(x))}{h^2} \, \tilde{\psi}(x, \nu) = 0$$

With $\hbar = h/2\pi$ we obtain the stationary Schrödinger equation

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By multiplying by $e^{-2\pi i\nu t}$, using $E = h\nu$ and integrating over ν:

$$\begin{aligned}
&-\tfrac{\hbar^2}{2m}\,\Delta\psi(x,t) + V(x)\psi(x,t)\\
&= \int e^{-2\pi i\nu t} h\nu\,\tilde{\psi}(x,\nu)d\nu = \frac{h}{-2\pi i}\int \frac{d}{dt}\left(e^{-2\pi i\nu t}\right)\tilde{\psi}(x,\nu)d\nu\\
&= i\hbar\frac{\partial}{\partial t}\,\psi(x,t)
\end{aligned}$$

The time dependent Schrödinger equation:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \Delta\psi(x,t) + V(x)\psi(x,t) \qquad (*)$$

- We have derived $(*)$ by an heuristic argument.
  From now on $(*)$ will be assumed;

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- $(*)$ is linear $\rightarrow$ interference phenomena;
- $\psi(x,t)$ is complex valued: not direct physical meaning;
- Conservation law: for ψ regular enough and decaying for large x, we have $\int_{\mathbb{R}^3} |\psi(x,t)|^2 dx = \int_{\mathbb{R}^3} |\psi(x,0)|^2 dx$.

Interpretation of the Schrödinger equation

Schrödinger: $\rho = e\,|\psi(x,t)|^2$ density of charge. But

- solutions of $(*)$ tipically spread in space as times goes by;
- a fraction of the electronic charge never observed.

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Statistical interpretation (Born, 1926)

$|\psi(x,t)|^2$ = probability density to find the microscopic particle in x at time t. For any measurable set A, $\int_A |\psi(x,t)|^2 dx =$ probability to find the particle in A at time t.

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$|\psi(x,t)|^2$ = probability density to find the microscopic particle in x at time t. For any measurable set A, $\int_A |\psi(x,t)|^2 dx =$ probability to find the particle in A at time t.

Suppose to perform N experiments in identical conditions, and denote with $N_{A,t}$ the number of times the particle is found in A at time t. Then: $\frac{N_{A,t}}{N} \xrightarrow[N \text{ large}]{} \int_A |\psi(x,t)|^2 dx$

Interpretation of the Schrödinger equation

Statistical interpretation: even if I completely know the state $\psi(x, t)$ what I can predict in general is only the probability/statistical distribution of results.

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Which is the meaning of this probability?

Might this probability be removed (hidden variables) or is it intrinsic?

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Is there a boundary among the classical and quantum description, and how to identify it?

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