MATHEMATICS OF QUANTUM MECHANICS

Lecturers: Davide Fermi and Massimo Moscolari
Exercise classes: Mattia Cantoni

Plan of the course

1) Introduction:
   - crisis of classical physics + wave/particle duality
   - reminders of CM + EM
   - Schrödinger formulation + von Neumann postulates

   $\Big\}$ ~ 3 lect.

2) Hilbert spaces and operator theory ~ 9 lect.

3) Basic models:
   - free particle
   - harmonic oscillator
   - hydrogen atom

   $\Big\}$ ~ 6 lect.

(+ 7 exercise lectures)

Bibliography

1. Lecture notes (on WeBeep).
2. M. Correggi, *Aspetti matematici della meccanica quantistica,* available at https://sites.google.com/view/michele-correggi/teaching
3. A. Teta, *A mathematical primer in quantum mechanics*, Springer (2018).
4. L.D. Landau, E.M. Lifshitz, *Quantum mechanics: non-relativistic theory* (*Course of theoretical physics*, vol. 3), Pergamon Press (1977).
5. M. Reed, B. Simon, *Functional analysis* (*Methods of modern mathematical physics, vol. 1),* Academic Press (1981).
6. F. Schwabl, *Quantum Mechanics,* Springer (1992).
7. Other references will be given during the course.

Exam

- Oral exam on the topics covered during the course.
- Presentation on a specific topic (to be agreed).

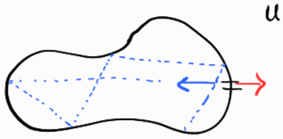
1. The crisis of classical physics

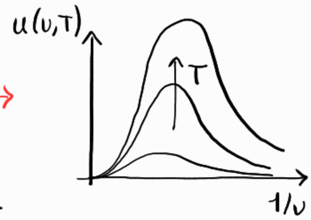
timeline of major physical theories:

1600 – 1800 : Classical Mechanics (Galileo, Newton, Lagrange, Hamilton, ...)
~ 1850 : Statistical Mechanics (Maxwell, Boltzmann, Gibbs, ...)
1873 : Electromagnetism (Maxwell, ...)
1900 - 1920 : Relativity (Einstein, Poincaré, Minkowski, ...)
1900 - 1940 : Quantum Mechanics (Planck, Einstein, Schrödinger, Bohr, Born, Dirac, Heisenberg, von Neumann, ...)

By the end of 1800, there was a strong belief that CM + EM could provide the ultimate and fundamental explanation of all physical phenomena.
this conviction was questioned by a series of unexpected experimental observations related to the behavior of cold/microscopic systems.

A) Black-body radiation





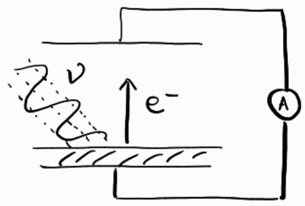
theoretical model proposed by Kirchhoff (1859)
think of a cavity with perfectly reflecting walls at fixed temperature

EM radiation enters passing through a small hole → it reaches thermal eq. with the walls → it gets re-emitted through the hole.

⇒ universality: internal EM energy density depends only on frequency and temperature (not on location/walls material and shape/polarization, ...).

- Wien (1896): EM radiation as a gas of particles ⇒ $u(\nu,T) \sim A\nu^3 e^{-c\nu/T}$
  Correct for $\nu \to \infty$
- Rayleigh-Jeans (1900-1905): EM radiation as stationary waves (equiv. decoupled harmonic oscillators) ⇒ $u(\nu,T) \sim B\nu^2 T$
  correct for $\nu \to 0$ // UV catastrophe: $\int_0^\infty d\nu\, u(\nu,T) = \infty$
- Planck (1900): energy can be exchanged only in discrete units ⇒ $u(\nu,T) \sim \frac{\nu^3}{e^{h\nu/k_B T} - 1}$
  Perfect agreement with experiment for $h = 6.6 \times 10^{-34}\ kg\, m^2/s = [\text{action}]$
  Total energy $U(T) = \int_0^\infty d\nu\, u(\nu,T) = \frac{c}{h^4}(k_B T)^4$ (Stefan-Boltzmann law)

B) Photoelectric effect



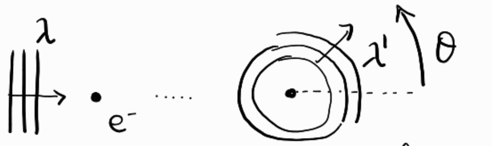
When a metallic surface is hit by monocromatic EM radiation of frequency ν, it emits electrons e^-:

- e^- emitted only if $\nu > \nu_0$, for some threshold frequency ν_0;
- maximum kinetic energy of emitted $e^- \propto \nu - \nu_0$ (linear);
- #(emitted e^-) $\propto$ intensity of EM radiation (NB: intensity does not affect velocity).

- Hertz (1887): experimental observation
- Einstein (1905): EM radiation formed by "quanta" of energy $h\nu$, which either get absorbed by the metal plate or do not interact at all. → energy is quantized, not EM radiation
  - e^- emitted only if $h\nu > h\nu_0 = E_0$ = single atom extraction energy;
  - maximum kinetic energy $= h\nu - E_0$;
  - e^- emitted by interaction of a single energy quantum ⇒ #(emitted e^-) $\propto h\nu \cdot N$

c) Compton effect

Consider a beam of X rays (monocromatic EM wave) getting scattered by a gas/ liquid sample.



- CM + EM: incident plane wave and scatterd spherical wave have the same wavelength
- Compton (1923): experimental observation $\lambda - \lambda' = a(1-\cos\theta)$ (*)

  theoretical explanation: Einstein's light quanta carry a momentum like classical particles. The relation (*) can be explained in terms of relativistic elastic scattering between a single (massless) light quantum ($\rightsquigarrow$ photon) and a single electron:

$$\lambda - \lambda' = \frac{h}{m_e c}(1-\cos\theta) \qquad \begin{pmatrix} h = \text{Plank constant} \\ c = \text{speed of light} \\ m_e = \text{electron mass} \end{pmatrix}$$

$\boxed{\begin{array}{l} \text{Rmk: } E = h\nu = \hbar\omega \\ \quad + \text{Special relativity} \\ \quad \hookrightarrow p = \hbar k \end{array}}$

Rmk (wave/particle duality) A, B, C show that, depending on the context, light behaves sometimes like a wave and others like a particle.

D) Atomic structure / emission and absorption spectra

When a monoatomic gas is hit by a light beam, EM radiation gets absorbed and re-emitted only for very specific frequencies.

- Balmer (1855): $\nu_{m,n} = c R_H \left(\frac{1}{m^2} - \frac{1}{n^2}\right)$, $m, n \in \mathbb{N}$, $m < n$. (R_H = Rydberg's const.)
- Perrin (1901): planetary model, without EM (unable to explain Balmer's result);
- Thomson (1904): plum pudding model (disproved by Geiger-Mardsen in 1909);
- Rutherford (1911): planetary model, with EM (explains scattering data but fails with EM: accelerated charge should radiate energy and fall to the center).
- Bohr (1913): 0. dimensional consideration:

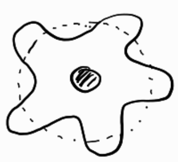
$$\frac{h}{m_e c^2} = [\text{length}] = 10^{-10}\,\text{m} = \text{atomic radius of hydrogen}$$

  1. $\exists$ priviledged classical orbits where the electron does not emit EM rad.
  $$E = -\frac{1}{2} h \nu_e \cdot n \qquad (\nu_e = e^- \text{ revolution frequency}, \ n \in \mathbb{N})$$
  2. EM radiation gets absorbed/emitted only if
  $$\nu_{EM} = |E_i - E_f| / h \qquad (E_{i/f} = \text{energy of stationary orbits})$$
  3. [angular momentum] = [action] $\rightarrow$ $|\vec{L}| = \hbar \cdot n$ $\left(\hbar = \frac{h}{2\pi}, \ n \in \mathbb{N}\right)$ ← Bohr-Sommerfeld quantization of constants of motion

  $\Rightarrow$ explains Balmer's formula. (Exercise - Correggi's notes)
- de Broglie (1924): e^- should be described by "waves of matter"

  Bohr's orbits match stationary waves (periodic b.c.)

  $\Rightarrow$ quantization of frequencies

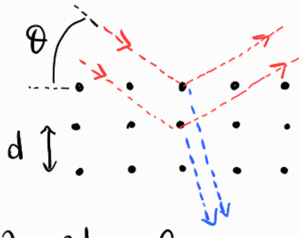


E) Diffraction of particles

A beam of electrons/neutrons hitting a crystal behaves like a wave with wavelength $\lambda = h/p$ (p = particles' classical momentum)

In particular, they follow Bragg's law for constructive interference

- Davisson-Germer (1927): experimental observation



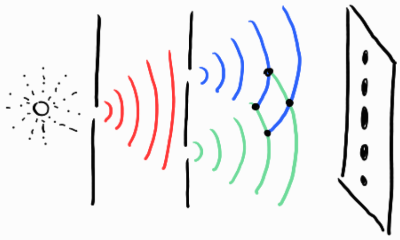
$\lambda = \frac{2d}{n}\sin\theta$,

$p = \hbar k$, $k = \frac{2\pi}{\lambda}$

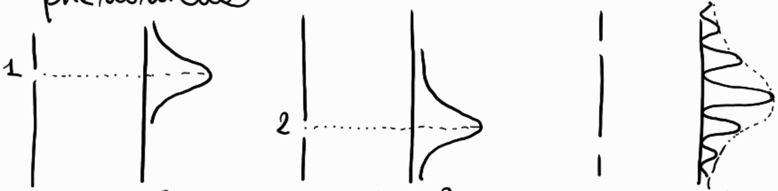
Rmk (wave/particle duality): Particles can behave like waves too!

F) Double slit experiment

- Young (1802): light is a wave and constructive/destructive superposition is responsible for interference phenomena

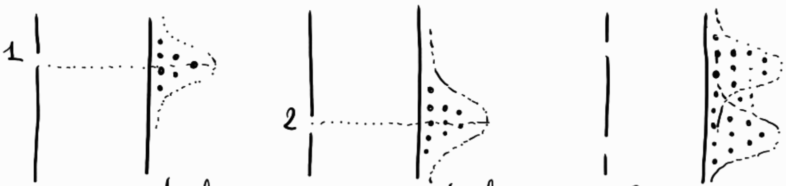


1. Waves:



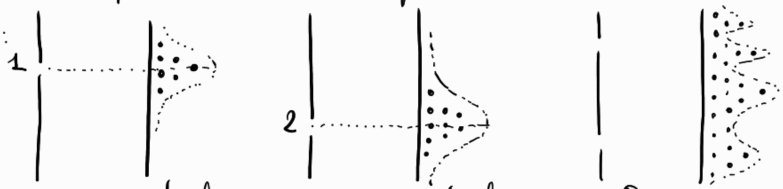
$I_1 = |A_1|^2$ $\quad$ $I_2 = |A_2|^2$ $\quad$ $I_{1+2} = |A_1 + A_2|^2$ $\rightarrow$ light intensity

2. Particles (classical):



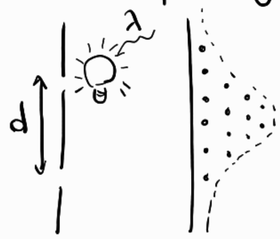
$P_1 = \#$ particles $\quad$ $P_2 = \#$ particles $\quad$ $P^c_{1+2} = P_1 + P_2$ $\rightarrow$ probability distrib. for particles

3. Electrons:



$P_1 = \#$ particles $\quad$ $P_2 = \#$ particles $\quad$ $P^Q_{1+2} \neq P_1 + P_2$ $\rightarrow$ counting particles produces a interference pattern!

Rmk: the pattern P^Q_{1+2} occurs even if electrons are emitted one at a time, so each electron is sort of making interference with itself. this can only occur if each electron passed through both slit 1 and 2. On the other side, electrons in cloud chambers produce classical trajectories. To make things even messier, the interference pattern P^Q_{1+2} reduces to P^c_{1+2} if one observes through which slit did the electrons pass, e.g. by putting a photodetector behind one of the slits.



When the photodetector wavelength λ is comparable with the interslit distance, it still produces a flash but it is impossible to tell through which slit the electron passed. In this case, the interference pattern reappears on the screen.

- Einstein (1927 - Solvay congress) proposed this as a gedankenexperiment.
- Jönsson (1961): interference pattern using electron beams.
- Merli, Missiroli, Pozzi (1974): 1 electron at a time, with a biprism replacing the double slit setting.
- Tonomura (1989, at Hitachi): 1 electron at a time, double slit ⤳ see video

References

1. P. Caldirola, R. Cirelli, G.M. Prosperi, *Introduzione alla fisica teorica, ch. IV,* UTET (1982).
2. M. Correggi, *Aspetti matematici della meccanica quantistica, ch. 1.*
3. R. Feynman, R. Leighton, M. Sands, *The Feynman lectures on physics, vol. 3, ch. 1,* Addison-Wesley (1964-1966).
4. A. Teta, *A mathematical primer in quantum mechanics, ch. 2,* Springer (2018).

2. Classical mechanics and electromagnetism

By the end of 1800, all accepted physical models rest on two key pillars:

- Classical Mechanics (Newton, Lagrange, Hamilton);
- Electromagnetism (Maxwell).

2.1 Classical mechanics

▸ Newton theory: 3 fundamental principles yielding the eq. of motion

$$\begin{cases} m\ddot{x} = F(x,\dot{x},t) \\ x(0) = x_0 \\ \dot{x}(0) = v_0 \end{cases} \rightarrow \text{ Cauchy problem for 2nd order ODE } \Rightarrow \text{ If } F \text{ is regular enough, then } \exists!\text{ solution } \forall t \in \mathbb{R}.$$

Rmk: Solution univocally determined by initial data (x_0, v_0) ⇒ determinism
Each particle is uniquely identified by its trajectory $t \mapsto x(t)$.

▸ Lagrange formulation:

Every mechanical system with n degrees of freedom can be described using an n-dimensional manifold M (space of configurations)

$$\begin{cases} q = (q_1, \dots, q_n) : U \subset M \to \mathbb{R}^n \\ \dot{q} = (v_1, \dots, v_n) \in \mathbb{R}^n \end{cases}$$
are coordinates on the tangent bundle TM (in simple cases $M = \mathbb{R}^n$, $TM = \mathbb{R}^n \times \mathbb{R}^n$).

The dynamics is encoded in a function (Lagrangian) $L : TM \times \mathbb{R}_t \to \mathbb{R}$, such that Newton's eq. match the Euler-Lagrange eq.

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \qquad \forall i = 1, \dots, n$$

Example: Consider a point particle in $\mathbb{R}^3$, subject to a conservative force $\bar{F}$.

$M = \mathbb{R}^3 \ni \bar{x}$, $TM = \mathbb{R}^3 \times \mathbb{R}^3 \ni (\bar{x}, \dot{\bar{x}})$

$\nabla \wedge \bar{F} = \bar{0}$ ($\mathbb{R}^3$ simply connected) $\Rightarrow \exists V : \mathbb{R}^3 \to \mathbb{R}$ s.t. $\bar{F} = -\nabla V$

$L(\bar{x}, \dot{\bar{x}}) = T - V = \frac{1}{2} m |\dot{\bar{x}}|^2 - V(\bar{x})$ (Exercise: write the EL eqs.)

Related developments:

- same EL eqs. for L and $L' = L + \frac{df}{dt}$;
- the mechanical energy $\mathcal{E}(q, \dot{q}, t) = \frac{\partial L}{\partial \dot{q}} \cdot \dot{q} - L \Rightarrow \frac{d\mathcal{E}}{dt} = -\frac{\partial L}{\partial t}$ (along solutions of EL eqs.)
  ⇒ conserved in autonomous syst.;
- If L is non-degenerate $\left(\det \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} \neq 0\right)$, EL eqs. $\Leftrightarrow \begin{cases} \dot{q} = v \\ \frac{d}{dt}\frac{\partial L}{\partial v} = \frac{\partial L}{\partial q} \end{cases}$ (system of 2n 1st order ODE);
- least action principle for $S^{q_0, q_1}_{t_0, t_1}[q] = \int_{t_0}^{t_1} dt\, L(q(t), \dot{q}(t), t)$;
- Noether theorem (symmetries ⟷ conservation laws);
- theory of small oscillations.

▸ Hamilton formulation

This formalism relies on the Legendre transform to highlight the symplectic structure of the theory:

a) $TM \ni (q, \dot{q})$ (tangent bundle) $\longrightarrow$ $T^*M \ni (q, p)$ (co-tangent bundle); "phase space"

b) $L(q, \dot{q}, t)$ (Lagrangian) $\longrightarrow$ $H(q, p, t) = \sup_{\dot{q} \in \mathbb{R}^n} \left[p \cdot \dot{q} - L(q, \dot{q}, t) \right]$ (Hamiltonian)

If L is non-deg., the extremal $\dot{q}$ is determined by $p = \frac{\partial L}{\partial \dot{q}}$ (inverse function thm)

c) EL eqs $\longrightarrow \begin{cases} \dot q = \frac{\partial H}{\partial p} \\ \dot p = -\frac{\partial H}{\partial q} \end{cases}$ (Hamilton eqs.) $\Longleftrightarrow$ $\dot z = J\,\nabla_z H = X_H(z,t)$ → Hamiltonian vector field

$z=(q,p)$, $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ = symplectic matrix

the solution of H. eqs. are the integral lines of X_H.

d) Mechanical energy $\mathcal{E}(q,\dot q,t)$ $\longrightarrow$ $\mathcal{E}(q,\dot q(q,p,t),t) = H(q,p,t)$

with $\frac{dH}{dt} = \cancel{\frac{\partial H}{\partial q}\dot q} + \cancel{\frac{\partial H}{\partial p}\dot p} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}$

Example: Consider a point particle in $\mathbb{R}^3$, subject to a conservative force $\bar F$.

$M = \mathbb{R}^3 \ni \bar x$, $\quad T^*M = \mathbb{R}^3 \times \mathbb{R}^3 \ni (\bar x, \bar p)$

$H(\bar x,\bar p) = T + V = \frac{1}{2m}|\bar p|^2 + V(\bar x)$ $\quad (\bar p = m\dot{\bar x})$ $\quad$ (Exercise: write the H. eqs.)

Related developments

- Liouville's thm: the Hamiltonian flows preserves volumes in phase space $(\nabla\cdot X_H = 0)$;
- Poincaré recurrence thm ($\rightsquigarrow$ Maxwell's demon);
- For any given function on phase space, there holds

$$\frac{d}{dt}F(q(t),p(t)) = \frac{\partial F}{\partial q}\cdot\dot q + \frac{\partial F}{\partial p}\cdot\dot p = \frac{\partial F}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial F}{\partial p}\frac{\partial H}{\partial q} = \{F,H\} \quad \text{(Poisson brackets)}$$

In particular: – F is a constant of motion iff. $\{F,H\} = 0$

– fundamental relations $\{q_i,q_j\} = \{p_i,p_j\} = 0$, $\{q_i,p_j\} = \delta_{ij}$ (Kronecker delta)

(Exercise: $\bar L = \bar q \wedge \bar p \in \mathbb{R}^3 \Rightarrow \{L_i,L_j\} = \sum_k \varepsilon_{ijk} L_k$) → Levi-Civita symbol

- Canonical transformation are maps $(q,p)\in T^*M \to (Q,P)\in T^*M$ such that
  1) $\dot q = \frac{\partial H}{\partial p}$, $\dot p = -\frac{\partial H}{\partial p} \Rightarrow \dot Q = \frac{\partial K}{\partial P}$, $\dot P = -\frac{\partial K}{\partial Q}$ for some $K: T^*M \to \mathbb{R}$;

  $\Updownarrow$

  2) $\{F,G\}_{q,p} = \{F,G\}_{Q,P}$ for all $F,G: T^*M \to \mathbb{R}$ $\quad (\{Q_i,P_j\} = \delta_{ij})$;

  $\Updownarrow$

  3) $p\,dq - H\,dt = c\,(P\,dQ - K\,dt) + dF$ (Poincaré-Cartan 1-form).
- Hamilton-Jacobi eq.: $\frac{\partial S}{\partial t} + H(q, \frac{\partial S}{\partial q}, t) = 0$
- Action/angle variables $\rightsquigarrow$ KAM theory

  Poincaré thm: If H is non-deg., generic, then $\nexists$ analytic constants of motion.

▸ States and observables in CM

Pure states are points in phase space: $(q,p)\in T^*M$

Rmk: It is assumed that positions/momenta can be measured with arbitrary precision.

Observables are functions on phase space: $F \in \mathcal{C}^1(T^*M;\mathbb{R})$

Rmk: $(\mathcal{C}^1(T^*M;\mathbb{R}),\cdot)$ with the pointwise product $(F\cdot G)(q,p) = F(q,p)\cdot G(q,p)$ is an associative, commutative and unital $\mathbb{R}$-algebra.

$(\mathcal{C}^1(T^*M,\mathbb{R}),\{\cdot,\cdot\})$ is a Lie algebra → bilinear, antisymmetric, Jacobi identity.

$\Rightarrow (\mathcal{C}^1(T^*M,\mathbb{R}),\cdot,\{\cdot,\cdot\})$ is a Poisson algebra

Rmk: The time evolution of a pure state is given by the Hamiltonian flow

$$\Phi^H_{t_0,t} \equiv \phi_t : T^*M \longrightarrow T^*M$$
$$(q_0,p_0) \longmapsto \phi_t(q_0,p_0) = (q(t),p(t)) = \text{solution of H. eqs. with initial data } (q_0,p_0)$$

The time evolution of an observable is given by

$$F(q(t),p(t)) = F(\phi_t(q_0,p_0)) = (F\circ\phi_t)(q_0,p_0) \equiv F_t(q_0,p_0)$$

↳ Schrödinger repres. Heisenberg repres.

Mixed states are probability densities on phase space ($\mu\geq 0$, $\int_{T^*M}\mu\, dq\,dp = 1$) the average value and std deviation of an observable are

$$\langle F\rangle_\mu = \int_{T^*M} F\mu\, dq\,dp = \int F\,d\mu \qquad \langle \Delta F\rangle_\mu = \langle (F-\langle F\rangle_\mu)^2\rangle_\mu = \langle F^2\rangle_\mu - \langle F\rangle_\mu^2$$

Rmk: States are positive and normalized linear functionals on the (Poisson) algebra of observables $(\mathcal{C}^1(T^*M,\circ,\{\cdot,\cdot\}))$:

$$\omega_\mu : \mathcal{C}^1(T^*M,\mathbb{R}) \longrightarrow \mathbb{R}, \quad F \longmapsto \omega_\mu(F) := \int F\,d\mu \qquad \text{with} \quad \omega_\mu(F)\geq 0 \ \ \forall F\geq 0, \quad \omega_\mu(1) = 1$$

Such states form a convex set, with pure states as extremal points.

$$\omega_{(q,p)}(F) = F(q,p) = \int F\,d\mu_{(q,p)} \rightarrow \mu_{(q,p)}(q',p') = \delta(q'-q)\,\delta(p'-p)$$

Rmk: $\langle F_t\rangle_{\mu_0} = \int F_t(q,p)\mu_0(q,p)\,dq\,dp = \int F_0(\phi_t(q,p))\,\mu_0(q,p)\,dq\,dp = \int F_0(q',p')\,\mu_0(\phi_{-t}(q',p'))\,\overset{1}{\cancel{|J|}}\,dq'dp'$ ↳ Liouville thm

$$= \int F_0(q',p')\,(\mu_0\circ\phi_{-t})(q',p')\,dq'dp' \equiv \int F_0(q',p')\,\mu_t(q',p')\,dq'dp' = \langle F_0\rangle_{\mu_t}$$

$$\Rightarrow \frac{d}{dt}\mu_t(q,p) = \frac{d}{dt}\mu_0(\phi_{-t}(q,p)) = \frac{d}{dt}\mu_0(q(-t),p(-t)) = \frac{\partial\mu_0}{\partial q}(-\dot q) + \frac{\partial \mu_0}{\partial p}(-\dot p)$$

$$= -\left(\frac{\partial\mu_0}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial\mu_0}{\partial p}\frac{\partial H}{\partial q}\right)(q(-t),p(-t)) = -\{\mu_0,H\}\big|_{\phi_{-t}(q,p)} = -\{\mu_t,H\}$$

$$\Rightarrow i\frac{d}{dt}\mu_t = \mathcal{L}\mu_t \quad \text{Liouville eq. with } \mathcal{L} := i\{H,\cdot\}$$

2.2 Classical electrodynamics

Electromagnetic phenomena are described by Maxwell's eqs.

$$(1)\ \nabla\cdot\vec E = 4\pi\rho \qquad (3)\ \nabla\wedge\vec B - \frac{1}{c}\frac{\partial\vec E}{\partial t} = \frac{4\pi}{c}\vec J \qquad \text{non-homogeneous}$$

$$(2)\ \nabla\cdot\vec B = 0 \qquad (4)\ \nabla\wedge\vec E + \frac{1}{c}\frac{\partial \vec B}{\partial t} = \vec 0 \qquad \text{homogeneous}$$

(Heaviside – Gibbs formulation)

ρ = charge density, $\vec J$ = current density, $\vec E$ = electric field, $\vec B$ = magnetic field

$Q = \int_\Omega \rho\,dx$ = total charge, $\Delta Q = \int_{\partial\Omega}\vec J\cdot\hat n\,d\sigma$ = total charge flowing across $\partial\Omega$ per unit time.

Rmk: $\left.\begin{array}{l}\partial_t(1) + \nabla\cdot(3)\\ \nabla\cdot(\nabla\wedge\vec B) = 0\end{array}\right\} \Rightarrow (5)\ \partial_t\rho + \nabla\cdot\vec J = 0 \Rightarrow$ charge conservation

Rmk: For given sources $\rho,\vec J$, eqs. (1–4) are 8 scalar PDE with only 6 scalar unknowns, namely the components of $\vec E,\vec B$

$$0 = \nabla\cdot(3) = \nabla\cdot\left(\nabla\wedge\vec B - \frac{1}{c}\frac{\partial\vec E}{\partial t} - \frac{4\pi}{c}\vec J\right) = -\frac{1}{c}\frac{\partial}{\partial t}(\nabla\cdot\vec E - 4\pi\rho) = -\frac{1}{c}\frac{\partial}{\partial t}(1)$$

$$0 = \nabla\cdot(4) = \nabla\cdot\left(\nabla\wedge\vec E + \frac{1}{c}\frac{\partial\vec B}{\partial t}\right) = \frac{1}{c}\frac{\partial}{\partial t}(\nabla\cdot\vec B) = \frac{1}{c}\frac{\partial}{\partial t}(2)$$

$\Rightarrow$ (1), (2) hold true $\forall t > t_0$ if they are valid at $t = t_0$ → constraints on initial data

$$\text{M eq.} \Leftrightarrow \begin{cases}\partial_t\vec E = c\,\nabla\wedge\vec B - 4\pi\vec J, \quad \partial_t\vec B = -c\,\nabla\wedge\vec E\\ \vec E|_{t=0} = \vec E_0,\ \vec B|_{t=0} = \vec B_0 \text{ with } \nabla\cdot\vec E_0 = 4\pi\rho,\ \nabla\cdot\vec B_0 = 0\end{cases}$$

↳ well-posed Cauchy problem (6 eqs., 6 unknowns)

Rmk: Noting that $\nabla\wedge(\nabla\wedge\bar{a}) = \nabla(\nabla\cdot\bar{a}) - \Delta\bar{a}$, Maxwell eqs. imply

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\bar{E} = \frac{1}{c}\frac{\partial}{\partial t}\left(\nabla\wedge\bar{B} - 4\pi\bar{j}\right) = \nabla\wedge\left(\frac{1}{c}\frac{\partial\bar{B}}{\partial t}\right) - \frac{4\pi}{c^2}\frac{\partial\bar{J}}{\partial t} = \nabla\wedge(-\nabla\wedge\bar{E}) - \frac{4\pi}{c^2}\frac{\partial\bar{J}}{\partial t}$$

$$= -\left[\nabla(\nabla\cdot\bar{E}) - \Delta\bar{E}\right] - \frac{4\pi}{c^2}\frac{\partial\bar{J}}{\partial t} = \Delta\bar{E} - 4\pi\left(\nabla\rho + \frac{1}{c^2}\frac{\partial\bar{J}}{\partial t}\right)$$

$$\Rightarrow \begin{cases} \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\bar{E} - \Delta\bar{E} = -4\pi\left(\nabla\rho + \frac{1}{c^2}\frac{\partial}{\partial t}\bar{J}\right) \\ \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\bar{B} - \Delta\bar{B} = \frac{4\pi}{c}\nabla\wedge\bar{j} \end{cases}$$

Non-homog. wave eqs. for $\bar{E},\bar{B}$, so $\bar{E},\bar{B}$ may propagate also in vacuum

Rmk: EM fields carry energy

$$\left.\begin{array}{l} \bar{f} = \rho\bar{E} + \frac{1}{c}\bar{j}\wedge\bar{B} = \text{Lorentz force density} \\ \pi = \bar{v}\cdot\bar{f} = \frac{\bar{j}}{\rho}\cdot\bar{f} = \bar{j}\cdot\bar{E} = \text{power density} \\ u = \frac{1}{8\pi}\left(|\bar{E}|^2 + |\bar{B}|^2\right) = \text{energy density} \\ \bar{S} = \frac{c}{4\pi}\bar{E}\wedge\bar{B} = \text{Poynting vector} \end{array}\right\} \Rightarrow \begin{array}{c} \frac{d}{dt}\int_\Omega u\,dx = -\int_\Omega \pi\,dx - \int_{\partial\Omega}\bar{S}\cdot\hat{n}\,d\sigma \\ \Updownarrow \\ \partial_t u + \pi + \nabla\cdot\bar{S} = 0 \end{array}$$

(Exercise)

$\bar{E},\bar{B}$ decay faster than $\frac{1}{|\bar{x}|}$ for $|\bar{x}|\to\infty \Rightarrow \int_{\partial B_R(0)}\bar{S}\cdot\bar{n}\,d\sigma \xrightarrow{R\to\infty} 0$

" " slower " " " $\Rightarrow$ " $\;\;\not\xrightarrow{R\to\infty} 0$ (radiative fields)

Rmk: To study the Maxwell eqs. it is convenient to introduce the potentials $V, \bar{A}$ s.t.

$$\bar{E} = -\nabla V - \frac{1}{c}\frac{\partial}{\partial t}\bar{A} \qquad \bar{B} = \nabla\wedge\bar{A}$$

(Exercise: prove that such $V,\bar{A}$ exist)

- $\bar{E},\bar{B}$ are invariant under gauge transformations
$$(V,\bar{A}) \longmapsto \left(V - \frac{1}{c}\frac{\partial\phi}{\partial t}, \bar{A} + \nabla\phi\right) \text{ for any } \phi\in\mathcal{C}^2$$
- $$\left.\begin{array}{l} 0 = \nabla\cdot\bar{B} = \nabla\cdot(\nabla\wedge\bar{A}) \\ 0 = \nabla\wedge\bar{E} + \frac{1}{c}\frac{\partial\bar{B}}{\partial t} = \nabla\wedge\left(-\cancel{\nabla V} - \cancel{\frac{1}{c}\frac{\partial}{\partial t}}\bar{A}\right) + \frac{1}{c}\frac{\partial}{\partial t}\cancel{(\nabla\wedge\bar{A})} \end{array}\right\} \to$$ Homogeneous Maxwell eqs. are always valid

$$\left.\begin{array}{l} 4\pi\rho = \nabla\cdot\bar{E} = \nabla\cdot\left(-\nabla V - \frac{1}{c}\frac{\partial}{\partial t}\bar{A}\right) = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}V - \Delta V - \frac{1}{c}\frac{\partial}{\partial t}\left(\frac{1}{c}\frac{\partial}{\partial t}V + \nabla\cdot\bar{A}\right) \\ \frac{4\pi}{c}\bar{j} = \nabla\wedge\bar{B} - \frac{1}{c}\frac{\partial\bar{E}}{\partial t} = \dots = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\bar{A} - \Delta\bar{A} + \nabla\left(\frac{1}{c}\frac{\partial}{\partial t}V + \nabla\cdot\bar{A}\right) \end{array}\right\} \to$$ Non-homog. eqs are 4 PDE in 4 unknown

- Lorentz gauge: fix $\frac{1}{c}\frac{\partial V}{\partial t} + \nabla\cdot\bar{A} = 0 \Rightarrow \begin{array}{l} \frac{1}{c^2}\frac{\partial^2}{\partial t^2}V - \Delta V = 4\pi\rho \\ \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\bar{A} - \Delta\bar{A} = \frac{4\pi}{c}\bar{j} \end{array}$ decoupled wave eqs.
(used in special relativity)

Coulomb gauge: fix $\nabla\cdot\bar{A} = 0 \Rightarrow -\Delta V = 4\pi\rho$ (used in electrostatic)

- the Lagrangian density for EM is given by
$$\mathcal{L} = \frac{1}{8\pi}\left(|\bar{E}|^2 - |\bar{B}|^2\right) - \rho V + \bar{j}\cdot\bar{A}$$
(Exercise: write the associated EL eqs.)

Example: For a point particle of mass m, charge e, and assigned trajectory $\bar{q}(t)$:

$$\begin{array}{l} \rho(\bar{x},t) = e\,\delta(\bar{x} - \bar{q}(t)) \\ \bar{j}(\bar{x},t) = e\,\dot{\bar{q}}(t)\,\delta(\bar{x} - \bar{q}(t)) \end{array} \Rightarrow$$ Exact solutions of M. eqs. are given by Liénard-Wiechert advanced/retarded fields

Assuming $\sup_t |\bar{q}(t)| \ll |\bar{x}|$, $\sup_t |\dot{\bar{q}}(t)| \ll c$, we have the asymptotics

$$\left.\begin{array}{l} \bar{B}(\bar{x},t) = \frac{e}{4\pi c^2}\frac{1}{|\bar{x}|}\ddot{\bar{q}}\left(t - \frac{|\bar{x}|}{c}\right)\wedge\hat{x} + \dots \\ \bar{E}(\bar{x},t) = \bar{B}(\bar{x},t)\wedge\hat{x} + \dots \end{array}\right\rangle$$ radiative fields! $(\bar{E}\perp\bar{B})$

Notably, an electron moving around a nucleus is accelerating $(\ddot{\bar{q}} \neq \bar{0})$.
So, it produces radiative EM fields which subtract energy to the particle.
$\Rightarrow$ fall to the center $\Rightarrow$ impossible to explain stability of the atom!

So far we regarded $\rho, \bar{j}$ to be assigned and tryed to solve M eqs. for $\bar{E}, \bar{B}$.
(Find the EM fields generated by moving charges).

Conversely, one may consider assigned EM fields $\bar{E}, \bar{B}$ (with related potentials $V, \bar{A}$) and try to solve Newton eq. comprising a Lorentz force term

$$m\bar{a} = e\bar{F} + \frac{1}{c} e \bar{v} \wedge \bar{B} \quad \longleftrightarrow \quad L(\bar{q}, \dot{\bar{q}}) = \frac{1}{2} m |\dot{\bar{q}}|^2 - e(V + \dot{\bar{q}} \cdot \bar{A})$$

$$\longleftrightarrow \quad H(\bar{q}, \bar{p}) = \frac{1}{2m} \left|\bar{p} - \frac{e}{c}\bar{A}\right|^2 + eV$$

(Exercise: write Lagrange and Hamilton eqs.)

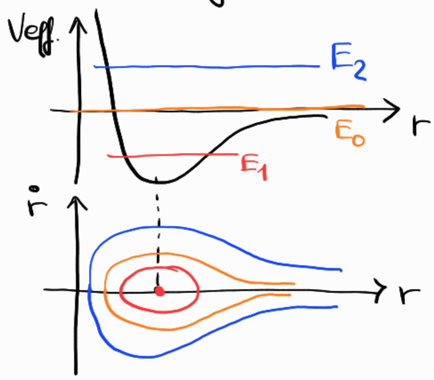
Example: For two point particles with opposite charges the Hamiltonian is

$$H(q_1, q_2; p_1, p_2) = \frac{1}{2m_1}|\bar{p}_1|^2 + \frac{1}{2m_2}|\bar{p}_2|^2 - \frac{e^2}{|\bar{q}_1 - \bar{q}_2|}$$

Factorizing the CM motion, one derives the reduced Hamiltonian

$$h(r, \theta; p_r, p_\theta) = \frac{1}{2\mu} p_r^2 + \frac{1}{2\mu}\frac{p_\theta^2}{r^2} - \frac{e^2}{r} = \frac{p_r^2}{2\mu} - V_{eff}(r)$$

the angular momentum p_θ and the total energy $E = h$ are constants of motion



$E_1 < 0 \rightarrow$ bounded orbits (bound states)

$E_0 = 0 \rightarrow$ separatrix

$E_2 > 0 \rightarrow$ unbounded orbits (scattering states)

- All energies $\geq \min V$ are allowed $\rightarrow$ in contrast with Bohmer rule
- If $p_\theta = 0$, $V_{eff} = -\frac{e^2}{r}$ is unbounded from below $\rightarrow$ fall to the center

Rmk: for point charges the Maxwell eqs. are always ill-defined due to UV issues (the electrostatic potential of a point-charge is too singular).
A possible way out is to solve the Maxwell eqs. for extended charges, solving at the same time the EM field eqs. and the motion of the charges
$\rightarrow$ Abraham model (semi-relativistic)
Lorentz model (relativistic)

References

1. P. Caldirola, R. Cirelli, G.M. Prosperi, *Introduzione alla fisica teorica, ch. I - III,* UTET (1982).
2. A. Teta, *A mathematical primer in quantum mechanics, ch. 1,* Springer (2018).
3. J.D. Jackson, *Classical electrodynamics,* Wiley (1962).
4. L.D. Landau, E.M. Lifshitz, *Course of theoretical physics*, vol. 1-2, Pergamon Press (1977).
5. H. Spohn, *Dynamics of charged particles and their radiation field, Cambridge University Press (2004).*

3. Introduction to quantum mechanics

The arguments outlined in the previous sections make evident that a new teory must be devised in order to study systems where the "characteristic action parameters" are small compared to $\hbar \sim 10^{-34}\, kg\, m/s^2$

- very small systems (atoms, molecules, ...);
- very cold systems (Bose-Einstein condensates, superconductors, ...)

(Exercise: determine the order of magnitude of the characteristic action parameters for a tabletop pendulum and for the classical hydrogen atom)

The historical development of Quantum Mechanics:

- Matrix mechanics: Heisenberg, Born, Jordan, Dirac (1925); Pauli derives the spectrum of the hydrogen atom (1926).
- Wave mechanics: de Broglie (1924), Schrödinger (1926).
- Axiomatic formulation: von Neumann (1932) $\rightsquigarrow$ Hilbert spaces formalism.
- Algebraic formulation: von Neumann, Jordan, Wigner (1934); Gelfand, Naimark, Segal (1945-1947); Haag (1964)

3.1 Guessing the Schrödinger equation

de Broglie's idea: particles can be described like waves in a matter field;
Schrödinger's ansatz: optical/mechanical analogy

Wave optics
EM wave's dynamics via wave eq: $\frac{1}{c^2}\partial_{tt}u - \Delta u = 0$

(1) $\downarrow$ $\lambda \to 0$ $(\nu \to \infty)$

Geometric optics
light rays dynamics via eikonal eq: $\partial_t f = \pm c|\nabla f|$

$\longleftrightarrow$

∃? Wave mechanics
Dynamical eq?

(2) $\downarrow$ $\lambda \to 0$ $(\nu \to \infty)$

Classical mechanics
particle dynamics via Hamilton-Jacobi eq: $\partial_t S = -H(q, \nabla S, t)$

(1) Consider a plane-wave solution of the wave eq: $u(t,x) = a(t,x)\, e^{if(t,x)/\lambda}$

$$0 = \frac{1}{c^2}\partial_{tt}u - \Delta u = \frac{1}{\lambda^2}\left[-\frac{1}{c^2}(\partial_t f)^2 + |\nabla f|^2\right] a\, e^{if/\lambda} + O\left(\frac{1}{\lambda}\right) \quad \text{for } \lambda \to 0^+$$

$\Rightarrow$ to leading order it must be fullfilled the eikonal eq: $\frac{1}{c}\partial_t f = \pm|\nabla f|$

Rmk: in geometric optics, $f \simeq$ action functional for geodesic paths.

(2) Schrödinger considered plane-waves of the form: $\Psi(t,x) = a(t,x)\, e^{iS(t,x)/\kappa}$

- S = classical action functional for a point particle $\to \partial_t S = -\left[\frac{1}{2m}|\nabla_x S|^2 + V\right]$
- κ = universal action constant $\rightsquigarrow \kappa = \hbar$.

$$\Rightarrow \begin{rcases} \text{(a) } \partial_t \Psi = \left[\partial_t a + \frac{i}{\kappa} a\, \partial_t S\right] e^{iS/\kappa} = -\frac{i}{\kappa}\left(\frac{1}{2m}|\nabla_x S|^2 + V\right)\Psi + O(1) \\ \text{(b) } \nabla_x \Psi = \left[\nabla_x a + \frac{i}{\kappa} a \nabla_x S\right] e^{iS/\kappa} = \frac{i}{\kappa}(\nabla_x S)\Psi + O(1) \\ \text{(c) } \Delta_x \Psi = \left[\Delta_x a + \frac{2i}{\kappa}\nabla_x a \cdot \nabla_x S + \frac{i}{\kappa} a\, \Delta_x S + a\left(\frac{i}{\kappa}\nabla_x S\right)^2\right] e^{iS/\kappa} = -\frac{1}{\kappa^2}|\nabla_x S|^2 \Psi + O\left(\frac{1}{\kappa}\right) \end{rcases} \text{for } \kappa \to 0^+$$

(a)+(c) $\Rightarrow$ $\boxed{ik\partial_t\Psi = -\frac{k^2}{2m}\Delta_x\Psi + V\Psi}$ Schrödinger's eq. (with $k=\hbar$)

(b) $\Rightarrow$ $\boxed{-ik\nabla_x\Psi = (\nabla_x S)\Psi = p\Psi}$ Momentum observable representation

Rmk: Formal translation: $(q,p)\longrightarrow(x,-i\hbar\nabla_x)$ and $H(q,p)\to -\frac{\hbar^2}{2m}\Delta_x + V$

Rmk: Schrödinger's eq. $\equiv$ PDE of order 1 in time

$\Rightarrow$ Fixing an initial datum $\Psi(t,x)|_{t=0} = \Psi_0(x)$ yields a well-posed Cauchy problem

$\Rightarrow$ deterministic evolution

Rmk: Schrödinger's eq. $\equiv$ complex PDE $\to$ complex-valued solutions Ψ

Rmk: Schrödinger's eq $\xrightarrow{\hbar\to 0^+}$ Hamilton-Jacobi eq.

$\hookrightarrow$ Wentzel-Kramers-Brillouin approximation.

Let us now proceed to examine the main consequences of the Schrödinger equation. Hereafter we limit ourselves to give a provisional mathematical analysis, deferring to the next chapters a fully rigorous discussion.

In the following, we systematically refer to the Schwarz space.

Def: The Schwarz space is $S = \{\Psi\in\mathcal{C}^\infty(\mathbb{R}^3,\mathbb{C}) \mid \sup_{x\in\mathbb{R}^3}|x^\alpha\partial_x^\beta\Psi|<\infty \ \ \forall\,\alpha,\beta\in\mathbb{N}^3 \text{ multi-indices}\}$

Rmk: $S \subsetneq \mathcal{C}^\infty(\mathbb{R}^3,\mathbb{C}) \subsetneq L^2(\mathbb{R}^3,\mathbb{C})$

$\uparrow$ functions which, together with all their derivatives, decay faster than any polynomial at infinity.

Rmk: S is a topological vector space (with Fréchet topology), which is closed w.r.t. pointwise product and derivation.

Rmk: S is not the optimal choice to study the Schrödinger eq. (it's too small!)

We henceforth assume that $\Psi(t,x)$ is a solution of

$$(Sc)\qquad i\hbar\,\partial_t\Psi(t,x) = -\frac{\hbar^2}{2m}\Delta_x\Psi(t,x) + V(x)\Psi(t,x) \qquad \forall\,(t,x)\in\mathbb{R}\times\mathbb{R}^3$$

Proposition: $\Psi(t,\cdot)\in S$ solution of (Sc) $\forall t>0$. Then

$$\|\Psi(t,\cdot)\|^2_{L^2(\mathbb{R}^3)} = \int_{\mathbb{R}^3}dx\,|\Psi(t,x)|^2 = \int_{\mathbb{R}^3}dx\,|\Psi(0,x)|^2 = \|\Psi(0,\cdot)\|^2_{L^2(\mathbb{R}^3)} \qquad \forall t>0.$$

proof: $\left.\begin{aligned}\overline{\Psi}\cdot(Sc) &\Rightarrow i\hbar\overline{\Psi}\partial_t\Psi = -\frac{\hbar^2}{2m}\overline{\Psi}\Delta\Psi + V|\Psi|^2\\ \Psi\cdot\overline{(Sc)} &\Rightarrow -i\hbar\Psi\partial_t\overline{\Psi} = -\frac{\hbar^2}{2m}\Psi\Delta\overline{\Psi} + V|\Psi|^2\end{aligned}\right\}\Rightarrow \begin{aligned}i\hbar\,\partial_t|\Psi|^2 &= -\frac{\hbar^2}{2m}(\overline{\Psi}\Delta\Psi - \Psi\Delta\overline{\Psi})\\ &= -\frac{\hbar^2}{2m}\nabla\cdot(\overline{\Psi}\nabla\Psi - \Psi\nabla\overline{\Psi})\end{aligned}$

$$\Rightarrow \frac{d}{dt}\int_{B_R(0)}dx\,|\Psi(t,x)|^2 = \int_{B_R(0)}dx\,\partial_t|\Psi(t,x)|^2 = \int_{B_R(0)}dx\,\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\right)\nabla\cdot(\overline{\Psi}\nabla\Psi-\Psi\nabla\overline{\Psi}) = \frac{i\hbar}{2m}\int_{\partial B_R(0)}d\sigma\,\hat{n}\cdot(\overline{\Psi}\nabla\Psi-\Psi\nabla\overline{\Psi}) \xrightarrow{R\to\infty} 0 \ \blacksquare$$

Rmk: Local conservation law

$\partial_t|\Psi|^2 - \frac{i\hbar}{2m}\nabla\cdot(\overline{\Psi}\nabla\Psi - \Psi\nabla\overline{\Psi}) = 0 \longrightarrow \begin{aligned}&\partial_t\rho + \nabla\cdot\vec{J} = 0,\\ &\rho = |\Psi|^2;\ \ \vec{J} = \tfrac{1}{2m}[\overline{\Psi}(-i\hbar\nabla\Psi) + h.c.]\end{aligned}$

Born interpretation (Bohr-Heisenberg - Copenhagen):

- electrons are always observed as point-like particles, but it is not possible to predict their position in a deterministic way.
- QM is intrinsecally non-deterministic, while the Schrödinger eq. is deterministic

↳ $|\psi(t,x)|^2$ = probability density for the electron position in $\mathbb{R}^3$ at time $t\in\mathbb{R}$.

probability normalization $\Leftrightarrow$ $1=\int_{\mathbb{R}^3} dx\,\rho = \int_{\mathbb{R}^3} dx\,|\psi|^2 = \|\psi(t,\cdot)\|^2_{L^2(\mathbb{R}^3)}$

(holds for all $t>0$ if it holds at $t=0$)

↳ For any given $\varphi\in L^2(\mathbb{R}^3)\setminus\{0\}$ one introduces $\psi=\varphi/\|\varphi\|_{L^2}$ s.t. $\|\psi\|_{L^2}=1$

↳ the probability of finding the electron in a given (measurable) space region $\Omega\subseteq\mathbb{R}^3$ at some given time $t>0$ is

$$\mathcal{P}(\Omega,t)=\int_\Omega dx\,|\psi(t,x)|^2=\int_{\mathbb{R}^3} dx\,\overline{\psi(t,x)}\,\mathbb{1}_\Omega(x)\,\psi(t,x) = (\psi,\mathbb{1}_\Omega\psi)_{L^2(\mathbb{R}^3)}$$

More precisely: repeating N times the same experiment measuring the position of one electron at a time, one would find the electron inside Ω at a given time $t>0$ for $N_\Omega\equiv N_\Omega(N)$ times. After many repetitions it is found that

$$\frac{N_\Omega}{N}\xrightarrow{N\to\infty}\int_\Omega dx\,|\psi(t,x)|^2$$

NB: In general, nothing is said about the position of a single electron. QM theory only predicts probabilities.

NB: the above arguments suggest that $L^2(\mathbb{R}^3,\mathbb{C})$, rather than S, is the natural space to discuss QM, at least for whatever concerns position measurements.

3.2 Considerations on the position and momentum of a Scrödinger particle

Let us now elaborate further on the formal correspondence $(q,p)\to(x,-i\hbar\nabla_x)$

Def: the position operator is $Q_\ell: S\to S$, $(Q_\ell\psi)(x)=x_\ell\psi(x)$;

the momentum operator is $P_\ell: S\to S$, $(P_\ell\psi)(x)=-i\hbar\frac{\partial}{\partial x_\ell}\psi(x)$.

Rmk: Q_ℓ, P_ℓ are symmetric w.r.t. the $L^2(\mathbb{R}^3;\mathbb{C})$-inner product. Namely, $\forall\varphi,\psi\in S$:

$$(\varphi,Q_\ell\psi)_{L^2}=\int_{\mathbb{R}^3}dx\,\overline{\varphi}(x)\,(Q_\ell\psi)(x)=\int_{\mathbb{R}^3}dx\,\overline{\varphi(x)}\,x_\ell\psi(x)=\int_{\mathbb{R}^3}dx\,\overline{(Q_\ell\varphi)(x)}\,\psi(x)=(Q_\ell\varphi,\psi)_{L^2};$$

$$(\varphi,P_\ell\psi)_{L^2}=\int_{\mathbb{R}^3}dx\,\overline{\varphi}(x)\,(-i\hbar\partial_\ell\psi)(x)\underset{\text{by parts}}{\overset{\text{integration}}{=}}\int_{\mathbb{R}^3}dx\,\overline{(-i\hbar\partial_\ell\varphi)(x)}\,\psi(x)=(P_\ell\varphi,\psi)_{L^2}.$$

Rmk: For any given $\psi\in L^2(\mathbb{R}^3;\mathbb{C})$ with $\|\psi\|_{L^2}=1$ yielding a probability density $|\psi(t,x)|^2$, the average values of position and momentum are given by

$$\langle Q_\ell\rangle_\psi=\int_{\mathbb{R}^3}dx\,|\psi(x)|^2x_\ell=\int_{\mathbb{R}^3}dx\,\overline{\psi(x)}\,x_\ell\psi(x)=(\psi,Q_\ell\psi)_{L^2}=\frac{(\psi,Q_\ell\psi)_{L^2}}{\|\psi\|^2_{L^2}},$$

P_ℓ symmetric and $\|\psi\|_{L^2}=1$

$$\langle P_\ell\rangle_\psi=\int_{\mathbb{R}^3}dx\,m\,j_\ell(x)=\int_{\mathbb{R}^3}dx\,\frac{1}{2}\left[\overline{\psi}(-i\hbar\nabla_\ell\psi)+\text{h.c.}\right]=\frac{1}{2}\left[(\psi,P_\ell\psi)+\text{h.c.}\right]=\frac{(\psi,P_\ell\psi)_{L^2}}{\|\psi\|^2_{L^2}}.$$

the corresponding standard deviations are given by

$$\langle\Delta Q\rangle^2_\psi:=\langle|\bar{Q}|^2\rangle_\psi-|\langle\bar{Q}\rangle_\psi|^2=(\psi,|\bar{Q}-\langle\bar{Q}\rangle_\psi|^2\psi)=\|(\bar{Q}-\langle\bar{Q}\rangle_\psi)\psi\|^2_{L^2}\geq0;$$

$$\langle\Delta P\rangle^2_\psi:=\langle|\bar{P}|^2\rangle_\psi-|\langle\bar{P}\rangle_\psi|^2=(\psi,|\bar{P}-\langle\bar{P}\rangle_\psi|^2\psi)=\|(\bar{P}-\langle\bar{P}\rangle_\psi)\psi\|^2_{L^2}\geq0.$$

<u>Proposition</u>: For any pair of operators $A,B: S\to S$ consider the <u>commutator</u>

$$[A,B] := AB - BA : S \to S.$$

then: $[Q_\ell,Q_k]\psi = 0,\ [P_\ell,P_k]\psi = 0,\ [Q_\ell,P_k]\psi = i\hbar\,\delta_{\ell k}\psi \quad \forall \psi\in S$

<u>proof</u>: $[Q_\ell,Q_k]=[P_\ell,P_k]=0$ follow trivially from $x_\ell x_k = x_k x_\ell$ and $\partial_\ell\partial_k\psi = \partial_k\partial_\ell\psi\ \forall\psi\in S$;

$$[Q_\ell,P_k]\psi = x_\ell(-i\hbar\partial_k\psi) - (-i\hbar\partial_k)(x_\ell\psi) = \cancel{x_\ell(-i\hbar\partial_k\psi)} - (-i\hbar\,\partial_k x_\ell)\psi - \cancel{x_\ell(-i\hbar\partial_k\psi)} = i\hbar\,\delta_{k\ell}\psi.$$

<u>Rmk</u>: the above commutation relations match the canonical Poisson brackets

$$\{q_\ell,q_k\}_{PB}=0,\quad \{p_\ell,p_k\}_{PB}=0,\quad \{q_\ell,p_k\}_{PB}=\delta_{\ell k}$$

$\{\cdot,\cdot\}_{PB}$ define an anti-symmetric product on the commutative algebra of smooth functions on phase space (namely, on classical observables);

$[\cdot,\cdot]$ define an anti-symmetric product on the non-commutative algebra of symmetric operators ($\rightsquigarrow$ quantum observables)

Canonical quantization: $\{\cdot,\cdot\}_{PB}$ in CM $\longrightarrow$ $\frac{1}{i\hbar}[\cdot,\cdot]$ in QM.

<u>Rmk</u>: For polynomial functions of positions (or momenta), building on the commutativity of the product $Q_\ell Q_k = Q_k Q_\ell$ (or $P_\ell P_k = P_k P_\ell$), it is natural to set

$$\Big(\sum_{\ell=1,2,3}\sum_{n_\ell\in\mathbb{N}} c_{\ell n} Q_\ell^{n_\ell}\Big)\psi(x) = \sum_\ell\sum_{n_\ell} c_{\ell n}\, x_\ell^{n_\ell}\psi(x)$$

$$\Big(\sum_{\ell=1,2,3}\sum_{n_\ell\in\mathbb{N}} c_{\ell n} P_\ell^{n_\ell}\Big)\psi(x) = \sum_\ell\sum_{n_\ell} c_{\ell n}\,(-i\hbar\,\partial_\ell)^{n_\ell}\psi(x) \qquad \text{for all } \psi\in S,$$

On the other hand, due to the non-commutativity of the mixed product $Q_\ell P_\ell \neq P_\ell Q_\ell$ there is an intrinsic ambiguity in the quantization of a generic classical observable:

$$q_\ell p_\ell = p_\ell q_\ell \text{ in CM} \overset{?}{\longleftrightarrow} Q_\ell P_\ell,\ P_\ell Q_\ell,\ \tfrac{1}{2}[Q_\ell P_\ell + P_\ell Q_\ell],\ \dots \text{ in QM ?}$$

(QM should be "more fundamental" than CM, yet different QM versions can reproduce the same CM theory in the appropriate limiting regime)

(Exercise: given $V(Q) = \sum_\ell\sum_{n_\ell} v_{\ell,n_\ell} Q_\ell^{n_\ell}$ with $v_{\ell,n_\ell}\in\mathbb{R}$, determine $[V(Q),P_k] = ?$)

<u>Proposition</u> (<u>Ehrenfest theorem</u>). Let $V\in C^1(\mathbb{R}^3)$ be a given potential

$\psi(t,\cdot)\in S$ solution $\forall t>0$ of $\quad i\hbar\,\partial_t\psi = -\frac{\hbar^2}{2m}\Delta_x\psi + V\psi \quad \Rightarrow \quad \begin{cases} \frac{d}{dt}\langle Q_\ell\rangle_{\psi(t)} = \frac{1}{m}\langle P_\ell\rangle_{\psi(t)} \\ \frac{d}{dt}\langle P_\ell\rangle_{\psi(t)} = -\langle \partial_\ell V(Q)\rangle_{\psi(t)} \end{cases}$

<u>proof</u>: $$\frac{d}{dt}\langle Q_\ell\rangle_{\psi(t)} = \frac{d}{dt}\int_{\mathbb{R}^3} dx\, x_\ell|\psi(t,x)|^2 = \int_{\mathbb{R}^3} dx\, x_\ell\,\partial_t\rho = \int_{\mathbb{R}^3} dx\, x_\ell(-\nabla\cdot\vec{j}) = \begin{pmatrix}\text{integration}\\ \text{by parts}\end{pmatrix} = \int_{\mathbb{R}^3} dx\,(\nabla x_\ell)\cdot\vec{j}$$

$$= \int_{\mathbb{R}^3} dx\,\frac{1}{2m}\big[\overline{\psi}(-i\hbar\partial_\ell\psi) + \text{h.c.}\big] = \frac{1}{2m}\big[(\psi,P_\ell\psi)_{L^2} + \text{h.c.}\big] = \frac{1}{m}(\psi,P_\ell\psi)_{L^2} = \frac{1}{m}\langle P_\ell\rangle_\psi$$

$$\frac{d}{dt}\langle P_\ell\rangle_{\psi(t)} = \frac{d}{dt}\int_{\mathbb{R}^3} dx\,\overline{\psi}(-i\hbar\partial_\ell\psi) = \int_{\mathbb{R}^3} dx\big[\overline{\partial_t\psi}(-i\hbar\partial_\ell\psi) + \overline{\psi}(-i\hbar\partial_\ell\partial_t\psi)\big] = \begin{pmatrix}\psi \text{ solution}\\ \text{of Sch. eq.}\end{pmatrix}$$

$$= \int_{\mathbb{R}^3} dx\Big[\overline{\tfrac{1}{i\hbar}\big(-\tfrac{\hbar^2}{2m}\Delta\psi + V\psi\big)}\Big](-i\hbar\partial_\ell\psi) + \overline{\psi}(-i\hbar\partial_\ell)\Big[\tfrac{1}{i\hbar}\big(-\tfrac{\hbar^2}{2m}\Delta\psi + V\psi\big)\Big] = \begin{pmatrix}\text{integrate } \Delta\\ \text{by parts}\end{pmatrix}$$

$$= \int_{\mathbb{R}^3} dx\Big[\Big(\cancel{-\tfrac{\hbar^2}{2m}\Delta\overline{\psi}} + V\overline{\psi}\Big)\partial_\ell\psi - \Big(\cancel{-\tfrac{\hbar^2}{2m}\Delta\overline{\psi}}\Big)\partial_\ell\psi - \overline{\psi}\,\partial_\ell(V\psi)\Big]$$

$$= \int_{\mathbb{R}^3} dx\Big[\cancel{V\overline{\psi}\partial_\ell\psi} - \overline{\psi}(\partial_\ell V)\psi - \cancel{\overline{\psi}V\partial_\ell\psi}\Big] = -(\psi,(\partial_\ell V)\psi)_{L^2} = -\langle\partial_\ell V\rangle_\psi \quad \blacksquare$$

Rmk: there is an evident analogy with the Newton eq. in CM. Yet, the matching is not exact, since in general:

$$\langle \partial_\ell V(Q)\rangle_\psi \neq \partial_\ell V(\langle Q\rangle_\psi) \qquad (*)$$

- Counterexample: $V(x) = a\, x_1^4 + b\, x_1^3 \;\to\; \partial_1 V(x) = 4a\, x_1^3 + 3b\, x_1^2$

  Take $\psi(x) = \psi(-x)$ even $\Rightarrow \langle \partial_1 V(Q)\rangle_\psi = \int_{\mathbb{R}^3} dx\, (\cancel{4a x_1^3} + 3b x_1^2)|\psi(x)|^2 = 3b\langle Q_1^2\rangle_\psi > 0$

  On the other side: $\langle Q_k\rangle_\psi = \int_{\mathbb{R}^3} dx\; x_k |\psi(x)|^2 = 0 \;\Rightarrow\; \partial_\ell V(\langle Q\rangle_\psi) = \partial_\ell V(0) = 0$
- the (missing) identity $(*)$ is always realized for quadratic potentials:

  $V(x) = a|\bar{x} - \bar{b}|^2 + c \;\Rightarrow\; \partial_\ell V(x) = 2a(x_\ell - b_\ell)$

  $\Rightarrow \langle \partial_\ell V\rangle_\psi = \langle 2a(Q_\ell - b_\ell)\rangle_\psi = 2a(\langle Q_\ell\rangle_\psi - b_\ell) = \partial_\ell V(\langle Q\rangle_\psi).$

Proposition (Heisenberg's uncertainty principle): For any given $\psi \in S$ with $\|\psi\|_{L^2} = 1$, the position and momentum standard deviations fulfill

$$\boxed{\langle \Delta Q\rangle_\psi \cdot \langle \Delta P\rangle_\psi \geq \frac{3}{2}\hbar}$$

proof: Without loss of generality, we may assume that $\langle Q\rangle_\psi = 0$, $\langle P\rangle_\psi = 0$. Then:

$$1 = \|\psi\|_{L^2}^2 = \left|\left(\psi, \frac{1}{3i\hbar}\sum_{\ell=1}^{3}[Q_\ell, P_\ell]\psi\right)_{L^2}\right| = \left|\frac{1}{3\hbar}\sum_\ell\left[(Q_\ell\psi, P_\ell\psi)_{L^2} - h.c.\right]\right| = \left|\frac{1}{3\hbar}\sum_\ell 2\,\mathrm{Im}(Q_\ell\psi, P_\ell\psi)\right|$$

$$\leq \frac{2}{3\hbar}\sum_\ell |(Q_\ell\psi, P_\ell\psi)| \underset{\text{Cauchy Schwarz}}{\leq} \frac{2}{3\hbar}\sum_\ell \|Q_\ell\psi\|_{L^2}\|P_\ell\psi\|_{L^2} \underset{\text{Cauchy Schwarz}}{\leq}$$

$$\leq \frac{2}{3\hbar}\left(\sum_\ell \|Q_\ell\psi\|_{L^2}^2\right)^{1/2}\left(\sum_\ell \|P_\ell\psi\|_{L^2}^2\right)^{1/2} = \frac{2}{3\hbar}\langle \Delta Q\rangle_\psi \langle \Delta P\rangle_\psi \qquad \blacksquare$$

Rmk: the position and momentum of a quantum particle cannot be measured simultaneously with infinite precision.

Exercise (Bohm's pilot wave)

$$\left.\begin{aligned} &\rho = |\psi|^2 = \text{probability density} \\ &\psi = |\psi|\, e^{i \arg\psi} \end{aligned}\right\} \Rightarrow \psi = \sqrt{\rho}\, e^{iS/\hbar} \to \text{Use the Schrödinger eq. to derive evolution eq.s for } \rho, S$$

3.3 The von Neumann postulates

The postulates we are going to present should not be intended as "mathematical axioms", but rather as "physical principles" (like Newton's one).

We shall introduce them in a preliminary form and defer to a later discussion their most general version.

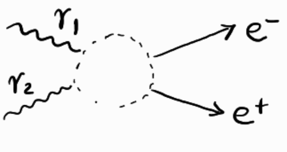
We firstly refer to the following "operative definitions"

- State of a system = result of a sequence of "substantial" manipulations/operations providing a suitable "preparation" of the system.

  (Two states coincide if the substantial conditions are the same)
- Observables ≡ measuring instruments which, upon interacting with the system, produce a numerical value ($\in \mathbb{R}, \mathbb{R}^n, \ldots$).

Rmk: No clear distinction between system and state.

Example:



(γ_1, γ_2) and (e^-, e^+) are two different states of the same system!

Rmk: No clear distinction between system and measuring apparatus
↳ at the core of decoherence and collapse problems.

Rmk: time and position of a state are not "substantial" properties of the system
↳ (Galilean) relativity $\longleftrightarrow$ reproducibility of experiments.

Rmk: time can be measured, but it is not a dynamical variable
↳ time $\equiv$ external parameter $t \in \mathbb{R}$.

Postulate 1 (States): A pure state is represented by a unit vector in a Hilbert space

$$\psi \in \mathcal{H} \quad \text{s.t.} \quad \|\psi\|_{\mathcal{H}} = 1.$$

Rmk: mixed states, composite systems, superselection rules will be discussed later on.

Rmk: $\mathcal{H}$ = complex Hilbert space

- Sóler thm: real / complex / quaternionic are the unique options.
- superposition principle: $\psi_1, \psi_2 \in \mathcal{H} \rightarrow \frac{\alpha\psi_1 + \beta\psi_2}{\|\alpha\psi_1 + \beta\psi_2\|}$ is an admissible state

  ↳ $\forall \psi \in \mathcal{H}$ represents a state (hypothesis).

Rmk: $\{$pure states$\}$ = $\{$unit vectors in $\mathcal{H}\}$ = $\{$rays in $\mathcal{H}\}$ = $\{$equivalence classes$\}$ = $(\mathcal{H}\setminus\{0\})/\sim$
with $\psi \sim \varphi$ iff $\psi = e^{i\alpha}\varphi$ for some $\alpha \in \mathbb{R}$.
$\Rightarrow$ $\{$pure states$\}$ = projective space $\rightarrow$ tricky to handle
↳ In practice: one works with vectors $\psi \in \mathcal{H}$, normalizing when necessary

Examples:
- $\mathcal{H} = (\mathbb{C}^n, \cdot_{st})$ with $(v,w)_{\mathbb{C}^n} = \overline{v} \cdot w = \sum_{\ell=1}^{n} \overline{v_\ell}\, w_\ell$
- $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C})$ with $(\varphi,\psi)_{L^2} = \int_{\mathbb{R}^3} dx\, \overline{\varphi(x)}\, \psi(x)$
- $\mathcal{H} = L^2(\Omega, \mathbb{C})$ with $(\varphi,\psi)_{L^2} = \int_{\Omega} dx\, \overline{\varphi(x)}\, \psi(x)$

Postulate 2 (observables): Admissible observables are represented by (unbounded) self-adjoint linear operators on the Hilbert space $\mathcal{H}$.

Rmk: $\{$observables$\} \subset \{$s.a. lin. oper. on $\mathcal{H}\} \equiv \mathcal{L}_{sa}(\mathcal{H})$
↳ It is not granted (though often understood) that any given $A \in \mathcal{L}_{sa}(\mathcal{H})$ actually represents an admissible observable.

Examples:
- $\mathcal{H} = \mathbb{C}^n$, $\mathcal{L}_{sa}(\mathcal{H})$ = Hermitian matrices $= \{A \in M_n(\mathbb{C}) \mid A = \overline{(A^T)} = A^* = A^\dagger\}$

> Spectral theorem (finite-dimensions): $\forall A \in \mathcal{L}_{sa}(\mathcal{H})$ $\exists \{b_1, \dots, b_n\}$ orthonormal base of eigenvectors with real eigenvalues $\{\lambda_1, \dots, \lambda_n\} \subset \mathbb{R}$ s.t.
>
> $$A b_\ell = \lambda_\ell b_\ell, \qquad (b_\ell, b_m)_{\mathbb{C}^n} = \delta_{\ell m}$$
>
> $$\Leftrightarrow \quad A = \lambda_1 \underbrace{\overline{b_1} \otimes b_1}_{= E_A(\lambda_1)} + \dots + \lambda_n \underbrace{\overline{b_n} \otimes b_n}_{= E_A(\lambda_n)} \longrightarrow \text{orthogonal projections on eigen-spaces}$$
>
> $\sigma(A) = \{\lambda_1, \dots, \lambda_n\} \subset \mathbb{R}$ is called the spectrum of A.

- $\mathcal{H} = L^2(\mathbb{R}^3)$, $Q_\ell = x_\ell$, $P_\ell = -i\hbar\partial_\ell$, $H = -\frac{\hbar^2}{2m}\Delta_x + V(x) \in \mathcal{L}_{sa}(\mathcal{H})$
- $\mathcal{H} = L^2(\Omega)$, $Q_\ell = x_\ell$, $H = -\frac{\hbar^2}{2m}\Delta_x + V(x) \in \mathcal{L}_{sa}(\mathcal{H})$

NB: In the last two examples one has to be careful about domains of definition
↳ regularity of V and boundary conditions on $\partial\Omega$ play a role.

<u>Postulate 3 (Dynamics)</u>: $\forall t \geq 0\ \exists H(t) \in \mathcal{L}_{sa}(\mathcal{H})$ "Hamiltonian operator" s.t. the time evolution of an initial state $\psi_0 \in \mathcal{H}$ is given by the solution of the Cauchy problem

$$\begin{cases} i\hbar \partial_t \psi = H(t)\psi \\ \psi(t)|_{t=0} = \psi_0 \end{cases}$$

<u>Rmk</u>: the existence of $H \in \mathcal{L}_{sa}(\mathcal{H})$ is a fundamental part of the postulate.

<u>Postulate 4 (Measurement)</u> [operative-verbal axiom]

a) When measuring an observable $A \in \mathcal{L}_{sa}(\mathcal{H})$, the possible numerical outcomes are the elements of the spectrum $\sigma(A) \subset \mathbb{R}$.

b) Given a system prepared in a state $\psi \in \mathcal{H}$, the probability that measuring an observable $A \in \mathcal{L}_{sa}(\mathcal{H})$ produces an outcome $\lambda \in I \subset \mathbb{R}$ is given by

$$\mathcal{P}_{A,\psi}(I) = (\psi, \underbrace{E_A(I)}_{\hookrightarrow \text{ spectral projector}}\psi)_{\mathcal{H}} = \| E_A(I)\psi\|^2_{\mathcal{H}}$$

c) If a value $\lambda \in I$ is observed upon measuring an observable $A \in \mathcal{L}_{sa}(\mathcal{H})$, then the state of the system "istantaneously" jumps to the state

$$\psi \xrightarrow{A} \tilde{\varphi} = \frac{E_A(I)\psi}{\|E_A(I)\psi\|}$$

<u>Example</u>: $\mathcal{H} = \mathbb{C}^n$, $A \in \mathcal{L}_{sa}(\mathcal{H}) \Rightarrow A = \lambda_1 E_A(\lambda_1) + \dots + \lambda_n E_A(\lambda_n)$, $E_A(\lambda_n)\psi = (b_n, \psi)_{\mathbb{C}^n} b_n$

$$\Rightarrow \mathcal{P}_{A,\psi}(\lambda_e) = (\psi, E_A(\lambda_e)\psi) = (\psi, (b_n,\psi)b_n) = (b_n,\psi)(\psi,b_n) = |(b_n,\psi)|^2 = \|E_A(\lambda_n)\psi\|^2$$

$= $ probability of transition from ψ to b_n.

$$\langle A\rangle_\psi = (\psi, A\psi) = (\psi, \sum_e \lambda_e E_A(\lambda_e)\psi) = \sum_e \lambda_e (\psi, E_A(\lambda_e)\psi) = \sum_e \lambda_e \mathcal{P}_{A,\psi}(\lambda_e)$$

$=$ average weighted with the transition probabilities.

<u>Rmk</u> (<u>Collapse of the wave-function</u>)

(P4c) $\Rightarrow$ istantaneous variation of the system

- Idea: measuring with a macroscopic apparatus produces a variation of the microscopic system
- Born: only statistical predictions can be derived
  No certain information about the single measurement.
- 2 different kinds of dynamics:
  P3 $\Rightarrow$ free (non-interacting) Schrödinger dynamics $\rightarrow$ deterministic
  P4 $\Rightarrow$ discontinuous and non-deterministic dynamics
  After the measurement has taken place, the system evolution is again ruled by the free dynamics:

$$\psi_0 \xrightarrow{P3} \psi(t) \overset{P4}{\rightsquigarrow} b_n \xrightarrow{P3} b_n(t).$$

References

1. M. Correggi, *Aspetti matematici della meccanica quantistica,* ch. 2.
2. B.C. Hall, Quantum Theory for Mathematicians, ch. 3, Springer (2013).
3. A. Teta, *A mathematical primer in quantum mechanics, ch. 3 and 5,* Springer (2018).