
Modern Physics

basics

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This material is part of the **basics-books project**. It is also available as a .pdf document.

Please check out the Github repo of the project, [basics-book project](#).

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Part I

Special Relativity

SPECIAL RELATIVITY

- Electromagnetism and the need for new relativity
- Space-time, Lorentz transformations,...
- Mechanics: kinematics, dynamics,...
- Electromagnetism: Maxwell's equations, potentials, Lorentz force, energy balance

SPECIAL RELATIVITY - NOTES

An event is determined by spatio-temporal information together, t, \vec{r} . Absolute nature of physics needs vector algebra and calculus formalism

$$\mathbf{X} = ct \mathbf{e}_0 + \vec{r} = ct \mathbf{e}_0 + x^1 \mathbf{e}_1 + x^2 \mathbf{e}_2 + x^3 \mathbf{e}_3 = X^\alpha \mathbf{E}_\alpha ,$$

having used Cartesian coordinates for the space coordinate.

Minkowski metric reads

$$g_{\alpha\beta} = \mathbf{E}_\alpha \cdot \mathbf{E}_\beta = \text{diag}\{-1, 1, 1, 1\}$$

The reciprocal basis reads $\mathbf{E}_\alpha \cdot \mathbf{E}^\beta = \delta_\alpha^\beta$, $\mathbf{E}_\alpha = g_{\alpha\beta} \mathbf{E}^\beta$, s.t. the elementary interval between two events can be written as

$$d\mathbf{X} = dX^\alpha \mathbf{E}_\alpha = \underbrace{dX^\alpha g_{\alpha\beta}}_{=dX_\beta} \mathbf{E}^\beta = dX_\beta \mathbf{E}^\beta ,$$

having used Cartesian coordinates,

$$\begin{array}{llll} X^0 = ct & X^1 = x & X^2 = y & X^3 = z \\ X_0 = ct & X_1 = -x & X_2 = -y & X_3 = -z \end{array}$$

Its “length”, or better pseudo-norm with Minkowski metric, is invariant and reads

$$ds^2 = d\mathbf{X} \cdot d\mathbf{X} = (dX_\alpha \mathbf{E}^\alpha) \cdot (dX^\beta \mathbf{E}_\beta) = c^2 dt^2 - (dx^1)^2 - (dx^2)^2 - (dx^3)^2 = c^2 dt^2 - |d\vec{r}|^2$$

Note: ds is invariant **todo** prove it. And/or add a section about the role of invariance.

For a co-moving observer, $d\vec{r}' = \vec{0}$, and t' is commonly indicated with τ , and its differential is invariant itself, being the product of a constant (c is a universal constant in special relativity) and an invariant quantity.

$$ds^2 = c^2 dt'^2 - |d\vec{r}'|^2 = c^2 d\tau^2 .$$

Given the invariant nature of ds ,

$$ds^2 = c^2 d\tau^2 = c^2 dt^2 - |d\vec{r}|^2 = c^2 dt^2 \left[1 - \frac{1}{c^2} \frac{|d\vec{r}|^2}{dt^2} \right] = c^2 dt^2 \left[1 - \frac{|\vec{v}|^2}{c^2} \right]$$

and thus

$$ds = c d\tau = \gamma^{-1}(v/c) c dt ,$$

with $\gamma(w) = \frac{1}{\sqrt{1-w^2}}$.

4-Velocity Given the parametric representation of an event in space-time as a function of its proper time, $\mathbf{X}(\tau)$ or coordinate s , $\mathbf{X}(s)$ the derivative w.r.t. this parameter is defined as the 4-velocity of the event in space time. Using Cartesian coordinates inducing constant and uniform basis \mathbf{E}_α , as a function of the observer time t , ct , $x^i(t)$, and the transformation of coordinates $t(\tau)$, with differential $dt = \frac{1}{\gamma} d\tau$

$$\mathbf{U}(\tau) := \mathbf{X}'(\tau) = \frac{d}{d\tau} (X^\alpha(\tau) \mathbf{E}_\alpha) = \frac{dt}{d\tau} (ct \mathbf{E}_0 + x^i(t) \mathbf{E}_i) = \gamma(v/c) (c \mathbf{E}_0 + \dot{x}^i(t) \mathbf{E}_i) = \gamma(v/c) (c \mathbf{E}_0 + \vec{v})$$

or

$$\mathbf{U}(s) := \mathbf{X}'(s) = \frac{dt}{ds} \frac{d}{dt} \mathbf{X}(t) = \dots = \gamma(v/c) \left(\mathbf{E}_0 + \frac{\vec{v}}{c} \right) .$$

Note: Using s as the parameter, \mathbf{U} is non-dimensional, and has pseudo-norm = 1,

$$\mathbf{U}(s) \cdot \mathbf{U}(s) = \gamma^2 \underbrace{\left(1 - \frac{|\vec{v}|^2}{c^2} \right)}_{=\gamma^{-2}} = 1 .$$

Using τ as the parameter, \mathbf{U} has physical dimension of a velocity and pseudo-norm = c .

4-acceleration $\mathbf{X}''(\tau)$ or $\mathbf{X}''(s)$, **todo**

2.1 Dynamics

4-momentum

$$\mathbf{P} = m\mathbf{U}$$

Using Cartesian coordinates and τ as independent variable,

$$\mathbf{P} = m\mathbf{U} = m \frac{d\mathbf{X}}{d\tau} = m\gamma(c, \vec{v}) .$$

The spatial component is γ times the 3-dimensional momentum $\vec{p} = m\vec{v}$; the time component reads

$$P^0 = m\gamma(w)c ,$$

and for small ratio $w := \frac{v}{c}$ it can be expanded in Taylor series around $w = 0$ as

$$\gamma(w) \sim \gamma(0) + w \gamma'(0) + \frac{1}{2} w^2 \gamma''(0) + o(w^2) ,$$

with

$$\begin{aligned} \gamma(w)|_{w=0} &= \frac{1}{\sqrt{1-w^2}} \Big|_{w=0} = 1 \\ \gamma'(w)|_{w=0} &= -\frac{1}{2} (1-w^2)^{-\frac{3}{2}} (-2w) \Big|_{w=0} = w(1-w^2)^{-\frac{3}{2}} = 0 \\ \gamma''(w)|_{w=0} &= \left((1-w^2)^{-\frac{3}{2}} + w \left(-\frac{3}{2} \right) (1-w^2)^{-\frac{5}{2}} (-2w) \right) \Big|_{w=0} = \\ &= \left((1-w^2)^{-\frac{3}{2}} + 3w^2 (1-w^2)^{-\frac{5}{2}} \right) \Big|_{w=0} = 1 \end{aligned}$$

and thus

$$\gamma(w) = 1 + \frac{1}{2}w^2 + o(w^2)$$

and

$$\gamma(v/c) m c \sim m c \left(1 + \frac{v^2}{c^2}\right) = \frac{1}{c} \left(mc^2 + \frac{1}{2}m|\vec{v}|^2\right)$$

Thus, recognizing energy ($E = \gamma mc^2$) and 3-momentum ($\vec{p} = m_3 \vec{v}$, with $m_3 := \gamma m$), the 4-momentum can be written as

$$\mathbf{P} = m\mathbf{U} = \gamma m \left(1, \frac{\vec{v}}{c}\right) =: \frac{1}{c} \left(\frac{E}{c}, \vec{p}\right)$$

Its pseudo-norm reads

$$m^2 = \mathbf{P} \cdot \mathbf{P} = \frac{1}{c^4} (E^2 - c^2 |\vec{p}|^2)$$

and thus the relation between E , \vec{p} , m and c ,

$$E^2 = m^2 c^4 + c^2 |\vec{p}|^2,$$

from which, for $\vec{v} = \vec{0} \rightarrow \vec{p} = \vec{0}$,

$$E^2 = m^2 c^4,$$

and keeping only the solution with positive energy (**todo** reference to Dirac's equation and anti-matter?)

$$E = mc^2.$$

2.1.1 Lagrangian approach

Free particle.

$$\mathbf{0} = \frac{d\mathbf{P}}{ds} = \frac{d}{ds} (m\mathbf{X}'(s))$$

Weak form

$$\begin{aligned} 0 &= \mathbf{W}(s) \cdot \frac{d}{ds} (m\mathbf{X}'(s)) = \\ &= \frac{d}{ds} [m\mathbf{W}(s) \cdot \mathbf{X}'(s)] - m\mathbf{W}'(s) \cdot \mathbf{X}'(s) = \end{aligned}$$

Using generalized coordinates $q^k(s)$, the event can be written in parametric form as $\mathbf{X}(q^k(s), s)$, while the velocity reads

$$\mathbf{U}(s) = \mathbf{X}'(s) = \frac{d}{ds} \mathbf{X}(q^k(s), s) = q^{k'}(s) \underbrace{\frac{\partial \mathbf{X}}{\partial q^k}(q^k(s), s)}_{= \frac{\partial \mathbf{X}'}{\partial q^k}} + \frac{\partial \mathbf{X}}{\partial s}(q^k(s), s) = \mathbf{U}(q^{k'}(s), q^k(s), s)$$

Choosing $\mathbf{W} = \frac{\partial \mathbf{X}}{\partial q^k} = \frac{\partial \mathbf{X}'}{\partial q^{k'}}$ in the weak form,

$$\begin{aligned} 0 &= \frac{d}{ds} [m\mathbf{W} \cdot \mathbf{X}'] - m\mathbf{W}' \cdot \mathbf{X}' = \\ &= \frac{d}{ds} \left[m \frac{\partial \mathbf{X}'}{\partial q^{k'}} \cdot \mathbf{X}' \right] - m \frac{d}{ds} \frac{\partial \mathbf{X}}{\partial q^k} \cdot \mathbf{X}' = \\ &= \frac{1}{2} \left[\frac{d}{ds} \left(\frac{\partial}{\partial q^{k'}} (m\mathbf{X}' \cdot \mathbf{X}') \right) - \frac{\partial}{\partial q^k} (m\mathbf{X}' \cdot \mathbf{X}') \right] = \end{aligned}$$

Defining

$$f(q^{k'}(s), q^k(s), s) = -m \mathbf{X}'(q^{k'}(s), q^k(s), s) \cdot \mathbf{X}'(q^{k'}(s), q^k(s), s) = -m ,$$

multiplying by a “regular” generic function $w(s)$, neglecting factor $\frac{1}{2}$ and integrating by parts

$$\begin{aligned} 0 &= - \int_{s=s_a}^{s_b} w(s) \left[\frac{d}{ds} \frac{\partial f}{\partial q^{k'}} - \frac{\partial f}{\partial q^k} \right] ds = \\ &= - \left[w(s) \frac{\partial f}{\partial q^{k'}} \right]_{s=s_a}^{s_b} + \int_{s=s_a}^{s_b} \left[w'(s) \frac{\partial f}{\partial q^{k'}} + \frac{\partial f}{\partial q^k} \right] ds = \\ &= - \left[w(s) \frac{\partial f}{\partial q^k} \right]_{s=s_a}^{s_b} + \delta \int_{s=s_a}^{s_b} f(q^{k'}(s), q^k(s), s) ds . \end{aligned}$$

Thus, provided that $w(s_1) = w(s_2) = 0$, equation of motion of free particle implies stationarity of functional

$$\int_{s=s_a}^{s_b} f(q^{k'}(s), q^k(s), s) ds ,$$

i.e.

$$\delta \int_{s=s_a}^{s_b} f(q^{k'}(s), q^k(s), s) ds = 0$$

Using t as independent parameter, $ds = \gamma^{-1} c dt$, the functional can be recast as

$$\int_{t=t_a}^{t_b} -m c \sqrt{1 - \frac{|\vec{v}|^2}{c^2}} dt ,$$

to find the (3-dimensional) Lagrangian (multiply by c to get the right physical dimension; check if it's required and wheter it's possible to make c appear before),

$$\mathcal{L} = -\sqrt{1 - \frac{|\vec{v}|^2}{c^2}} m c^2 ,$$

and retrieve 3-momentum as (being $\vec{v} = \dot{\vec{r}}$)

$$\begin{aligned} \vec{p} &:= \frac{\partial \mathcal{L}}{\partial \dot{\vec{r}}} = \\ &= -m c^2 \frac{1}{2} \left(1 - \frac{|\vec{v}|^2}{c^2} \right)^{-\frac{1}{2}} \left(-2 \frac{\vec{v}}{c^2} \right) = \\ &= m \left(1 - \frac{|\vec{v}|^2}{c^2} \right)^{-\frac{1}{2}} \vec{v} = \\ &= \gamma m \vec{v} , \end{aligned}$$

and energy as

$$\begin{aligned} E &:= \vec{p} \cdot \vec{v} - \mathcal{L} = \\ &= \gamma m |\vec{v}|^2 + \gamma^{-1} m c^2 = \\ &= \gamma m c^2 \left(\frac{|\vec{v}|^2}{c^2} + \gamma^{-2} \right) = \\ &= \gamma m c^2 \left(\frac{|\vec{v}|^2}{c^2} + 1 - \frac{|\vec{v}|^2}{c^2} \right) = \\ &= \gamma m c^2 . \end{aligned}$$

2.2 Electromagnetism

2.2.1 Classical electromagnetic theory

Maxwell equations

Maxwell equations read

$$\begin{cases} \nabla \cdot \vec{d} = \rho_f \\ \nabla \times \vec{e} + \partial_t \vec{b} = \vec{0} \\ \nabla \cdot \vec{b} = 0 \\ \nabla \times \vec{h} - \partial_t \vec{d} = \vec{j}_f \end{cases}$$

or in vacuum, with $\rho_f = \rho$, $\vec{j} = \vec{j}_f$, $\vec{d} = \varepsilon_0 \vec{e}$, $\vec{b} = \mu_0 \vec{h}$

$$\begin{cases} \nabla \cdot \vec{e} = \frac{\rho}{\varepsilon_0} \\ \nabla \times \vec{e} + \partial_t \vec{b} = \vec{0} \\ \nabla \cdot \vec{b} = 0 \\ \nabla \times \vec{b} - \mu_0 \varepsilon_0 \partial_t \vec{e} = \mu_0 \vec{j} \end{cases}$$

Electromagnetic potentials

The electromagnetic field can be written in terms of the electromagnetic potentials

$$\begin{cases} \vec{b} = \nabla \times \vec{a} \\ \vec{e} = -\partial_t \vec{a} - \nabla \varphi \end{cases}$$

Lorentz force

A particle in motion in a electromagnetic field is subject to Lorentz force. In classical electromagnetism, the expression of Lorentz force reads

$$\vec{F} = q \left(\vec{e} - \vec{b} \times \vec{v} \right) ,$$

whose power is

$$\vec{v} \cdot \vec{F} = \vec{v} \cdot q \left(\vec{e} - \vec{b} \times \vec{v} \right) = q \vec{v} \cdot \vec{e} .$$

2.2.2 Electromagnetic potential

$$\begin{cases} \vec{b} = \nabla \times \vec{a} \\ \vec{e} = -\partial_t \vec{a} - \nabla \varphi \end{cases}$$

$$\mathbf{A} = \mathbf{E}_\alpha A^\alpha = \frac{\varphi}{c} \mathbf{E}_0 + \vec{a}$$

$$\nabla \mathbf{A} = \left(\mathbf{E}^\alpha \frac{\partial}{\partial X^\alpha} \right) (A^\beta \mathbf{E}_\beta) = \frac{\partial A^\beta}{\partial X^\alpha} \mathbf{E}^\alpha \otimes \mathbf{E}_\beta = g_{\alpha\gamma} \frac{\partial A^\beta}{\partial X^\alpha} \mathbf{E}_\gamma \otimes \mathbf{E}_\beta .$$

whose components may be collected in a 2-dimensional array (first index for rows, second index for columns),

$$(\nabla \mathbf{A})_{\alpha}^{\beta} = \frac{\partial A^{\beta}}{\partial X^{\alpha}} = \begin{bmatrix} c^{-2} \partial_t \varphi & c^{-1} \partial_x \varphi & c^{-1} \partial_y \varphi & c^{-1} \partial_z \varphi \\ c^{-1} \partial_t a_x & \partial_x a_x & \partial_y a_x & \partial_z a_x \\ c^{-1} \partial_t a_y & \partial_x a_y & \partial_y a_y & \partial_z a_y \\ c^{-1} \partial_t a_z & \partial_x a_z & \partial_y a_z & \partial_z a_z \end{bmatrix}$$

or covariant-covariant components,

$$(\nabla \mathbf{A})_{\alpha\beta} = \frac{\partial A_{\beta}}{\partial X^{\alpha}} = g_{\beta\gamma} \frac{\partial A^{\gamma}}{\partial X^{\alpha}} = \begin{bmatrix} c^{-2} \partial_t \varphi & c^{-1} \partial_x \varphi & c^{-1} \partial_y \varphi & c^{-1} \partial_z \varphi \\ -c^{-1} \partial_t a_x & -\partial_x a_x & -\partial_y a_x & -\partial_z a_x \\ -c^{-1} \partial_t a_y & -\partial_x a_y & -\partial_y a_y & -\partial_z a_y \\ -c^{-1} \partial_t a_z & -\partial_x a_z & -\partial_y a_z & -\partial_z a_z \end{bmatrix}$$

or contravariant-contravariant components,

$$(\nabla \mathbf{A})^{\alpha\beta} = \frac{\partial A^{\beta}}{\partial X_{\alpha}} = g^{\beta\gamma} \frac{\partial A^{\alpha}}{\partial X^{\gamma}} = \begin{bmatrix} c^{-2} \partial_t \varphi & -c^{-1} \partial_x \varphi & -c^{-1} \partial_y \varphi & -c^{-1} \partial_z \varphi \\ c^{-1} \partial_t a_x & -\partial_x a_x & -\partial_y a_x & -\partial_z a_x \\ c^{-1} \partial_t a_y & -\partial_x a_y & -\partial_y a_y & -\partial_z a_y \\ c^{-1} \partial_t a_z & -\partial_x a_z & -\partial_y a_z & -\partial_z a_z \end{bmatrix}$$

The electromagnetic field tensor is defined as the anti-symmetric part of the gradient of the 4-electromagnetic potential,

$$\mathbf{F} = [\nabla \mathbf{A} - (\nabla \mathbf{A})^T]$$

whose components may be collected in a 2-dimensional array (first index for rows, second index for columns),

$$F^{\alpha\beta} = \begin{bmatrix} 0 & -\frac{e^T}{c} \\ \frac{e}{c} & \underline{b}_{\times} \end{bmatrix}, \quad F_{\alpha\beta} = \begin{bmatrix} 0 & \frac{e^T}{c} \\ -\frac{e}{c} & \underline{b}_{\times} \end{bmatrix}$$

2.2.3 Electromagnetic field and electromagnetic field equations

The pair of Maxwell equations

$$\begin{cases} \rho_f = \nabla \cdot \vec{d} \\ \vec{j}_f = -\partial_t \vec{d} + \nabla \times \vec{h} \end{cases}$$

can be re-written in 4-formalism, using 4-gradient in Cartesian coordinates

$$\nabla = \mathbf{E}^{\alpha} \frac{\partial}{\partial X^{\alpha}} = \mathbf{E}_0 \frac{\partial}{c \partial t} + \mathbf{E}_i \frac{\partial}{\partial x^i} = \mathbf{E}_0 \frac{\partial}{c \partial t} + \nabla,$$

and the definition of the 4-current density vector

$$\mathbf{J} = J^{\alpha} \mathbf{E}_{\alpha} = c\rho \mathbf{E}_0 + \vec{j}$$

so that

$$c\rho \mathbf{E}_0 + \vec{j} = \nabla \cdot \mathbf{F} = \nabla \cdot [(0 \mathbf{E}_0 + c\vec{d}) \otimes \mathbf{E}_0 + (-\mathbf{E}_0 c\vec{d} + \vec{h}_{\times})],$$

with the displacement field tensor,

$$\mathbf{D} = D^{\alpha\beta} \mathbf{E}_{\alpha} \mathbf{E}_{\beta},$$

with components (rows for the first index, columns for the second index)

$$D^{\alpha\beta} = \begin{bmatrix} 0 & -cd_x & -cd_y & -cd_z \\ cd_x & 0 & -h_z & h_y \\ cd_y & h_z & 0 & -h_x \\ cd_z & -h_y & h_x & 0 \end{bmatrix} = \begin{bmatrix} 0 & -c\underline{d}^T \\ \underline{cd} & \underline{h}_{\times} \end{bmatrix}$$

The pair of Maxwell equations

$$\begin{cases} \nabla \cdot \vec{b} = 0 \\ \partial_t \vec{b} + \nabla \times \vec{e} = \vec{0} \end{cases}$$

can be re-written in 4-formalism as

$$0 = \partial_\mu F_{\eta\xi} + \partial_\eta F_{\xi\mu} + \partial_\xi F_{\mu\eta}$$

Among these $64 = 4^3$ equations, there are only 4 independent equations.

- If 2 indices are the same, the corresponding equation is the identity $0 = 0$. As an example, if $\mu = \eta$

$$0 = \partial_\mu F_{\mu\xi} + \underbrace{\partial_\mu F_{\xi\mu}}_{-F_{\mu\xi}} + \underbrace{\partial_\xi F_{\mu\mu}}_{=0} = 0,$$

thus only combinations with different indices may provide some information.

- Given the ordered set of indices (μ, η, ξ) , switching a pair of indices provides the same equation. As an example, switching μ and η

$$\begin{aligned} 0 &= \partial_\eta F_{\mu\xi} + \partial_\mu F_{\xi\eta} + \partial_\xi F_{\eta\mu} = \\ &= \partial_\eta(-F_{\xi\mu}) + \partial_\mu(-F_{\eta\xi}) + \partial_\xi(-F_{\mu\eta}). \end{aligned}$$

- Thus, only 4 combination of different indices, without taking order into account, provide independent information

$$\begin{aligned} (1, 2, 3) : \quad 0 &= \partial_1 F_{23} + \partial_2 F_{31} + \partial_3 F_{12} = \partial_x(-b_x) + \partial_y(-b_y) + \partial_z(-b_z) \\ (2, 3, 0) : \quad 0 &= \partial_2 F_{30} + \partial_3 F_{02} + \partial_0 F_{23} = \partial_y\left(-\frac{e_z}{c}\right) + \partial_z\left(\frac{e_y}{c}\right) + \partial_{ct}(-b_x) \\ (3, 0, 1) : \quad 0 &= \partial_3 F_{01} + \partial_0 F_{13} + \partial_1 F_{30} = \partial_z\left(\frac{e_x}{c}\right) + \partial_{ct}(-b_y) + \partial_x\left(-\frac{e_z}{c}\right) \\ (0, 1, 2) : \quad 0 &= \partial_0 F_{12} + \partial_1 F_{20} + \partial_2 F_{01} = \partial_{ct}(-b_z) + \partial_x\left(-\frac{e_y}{c}\right) + \partial_y\left(\frac{e_x}{c}\right) \end{aligned}$$

i.e.

$$\begin{aligned} (1, 2, 3) : \quad 0 &= -\nabla \cdot \vec{b} \\ (2, 3, 0) : \quad 0 &= -\frac{1}{c} [\partial_t b_x + (\partial_y e_z - \partial_z e_y)] \\ (3, 0, 1) : \quad 0 &= -\frac{1}{c} [\partial_t b_y + (\partial_z e_x - \partial_x e_z)] \\ (0, 1, 2) : \quad 0 &= -\frac{1}{c} [\partial_t b_z + (\partial_x e_y - \partial_y e_x)] \end{aligned}$$

i.e.

$$\begin{cases} 0 = \nabla \cdot \vec{b} \\ \vec{0} = \partial_t \vec{b} + \nabla \times \vec{e} \end{cases}$$

2.2.4 Point particle in electromagnetic field

Lorentz 4-force acting on a point charge of electric charge q reads

$$\mathbf{f} = \mathbf{F} \cdot \mathbf{J} = q \mathbf{F} \cdot \mathbf{U}.$$

so that the dynamical equation reads

$$m \mathbf{X}'' = q \mathbf{F} \cdot \mathbf{X}'$$

2.2.5 Energy balance

$$\frac{\partial u}{\partial t} =$$
$$\frac{\partial \vec{s}}{\partial t} =$$

...

$$\nabla \cdot \mathbf{T} = -\mathbf{F} \cdot \mathbf{J}$$

Part II

General Relativity

GENERAL RELATIVITY

GENERAL RELATIVITY - NOTES

Part III

Statistical Mechanics

STATISTICAL PHYSICS

STATISTICAL PHYSICS - NOTES

6.1 Ensembles

6.2 Microcanonical ensemble

6.3 Canonical ensemble

6.4 Macrocanonical ensemble

6.5 Statistics

Each of the N components of the system is in an **energy level** i . Energy level i has g_i sublevels with the same energy level.

- energy levels, E_i of each component
- occupation number N_i of level i
- **Central role of energy.** In a system macroscopically at rest, the energy of a system is the only macroscopic meaningful non-zero mechanical quantity, constant for closed and isolated systems
- **Principle of maximum uncertainty, maximum entropy, minimum information:** given a measurement of a macroscopic variable V , describing the macrostate of the system, the feasible un-observed/able microstates of the system are the microstates consistent with it: there's usually a sharp maximum of in the probability density of the microstates.

Given a macrostate, what's the number of ways $W(N_i; g_i)$ to get a consistent microstate? Once the expression is found, constrained optimization follows: optimization w.r.t. N_i is usually performed in the limit of $N_i \rightarrow +\infty$ (why in Fermi-Dirac distribution, obeying Pauli exclusion principle?), with the values of the macroscopic variables as constraints usually treated with Lagrange multiplier.

6.5.1 Maxwell-Boltzmann

Statistics of distinguishable components.

6.5.2 Bose-Einstein

Statistics of undistinguishable components that can be in the same (sub)level. Given the number of elementary components $\sum_i N_i = N$ and the energy $\sum_i N_i E_i = E$,

$$W_{BE,i} = \frac{(N_i + g_i - 1)!}{N_i! (g_i - 1)!} \quad , \quad W_{BE} = \prod_i W_{BE,i} . \quad (6.1)$$

Counting microstates

todo write page *Combinatorics* and add link

Most likely microstate. Instead of maximizing (6.1), the objective function is $\ln W_{BE}$, after using Stirling approximation in the limit of large N_i and g_i , $N_i! \sim \left(\frac{N_i}{e}\right)^{N_i}$. The approximate occupation number of one of the G_i sublevels of the i^{th} level of the most likely microstate is

$$n_i := \frac{N_i}{G_i} = \frac{1}{e^{\alpha + \beta E_i} - 1} .$$

Optimization

$$\begin{aligned} J(N_i, \alpha, \beta) &= \ln W_{BE} + \alpha \left(N - \sum_i N_i \right) + \beta \left(E - \sum_i N_i E_i \right) = \\ &= \sum_i \{ \ln(N_i + g_i - 1)! - \ln N_i! - \ln(g_i - 1)! \} + \alpha \left(N - \sum_i N_i \right) + \beta \left(E - \sum_i N_i E_i \right) \simeq \\ &\simeq \sum_i \{ (N_i + g_i - 1) \ln(N_i + g_i - 1) - N_i \ln N_i - (g_i - 1) \ln(g_i - 1) + N_i + g_i - 1 - N_i - (g_i - 1) \} + \alpha \left(N - \sum_i N_i \right) + \beta \left(E - \sum_i N_i E_i \right) \\ &= \sum_i \{ (N_i + g_i - 1) \ln(N_i + g_i - 1) - N_i \ln N_i - (g_i - 1) \ln(g_i - 1) \} + \alpha \left(N - \sum_i N_i \right) + \beta \left(E - \sum_i N_i E_i \right) \end{aligned}$$

Using $\partial_n(n + a) \ln(n + a) = \ln(n + a) + 1$,

$$0 = \partial_{N_k} J \simeq \{ \ln(N_k + g_k - 1) - \ln N_k \} - \alpha - \beta E_k ,$$

and thus

$$\begin{aligned} \ln \frac{N_k + g_k - 1}{N_k} &= \alpha + \beta E_k , \\ \frac{N_k + g_k - 1}{N_k} &= e^{\alpha + \beta E_k} \\ N_k &= \frac{g_k - 1}{e^{\alpha + \beta E_k} - 1} \simeq \frac{g_k}{e^{\alpha + \beta E_k} - 1} , \end{aligned}$$

Thus, in the limit of $g_k \gg 1$, the occupation number of the k level is

$$N_k = \frac{G_k}{e^{\alpha + \beta E_k} - 1} ,$$

and the average occupation number of one of the g_k sublevels in the k level is

$$n_k := \frac{N_k}{G_k} = \frac{1}{e^{\alpha + \beta E_k} - 1}$$

Meaning of α, β

Example 1 (Black-body radiation: Planck, Wien, and Stefan-Boltzmann laws)

Planck's law. Energy density w.r.t. frequency

$$u_f(f, T) = \frac{8\pi h f^3}{c^3} \frac{1}{e^{\frac{hf}{k_B T}} - 1}$$

Planck's law in a cubic box

Planck's law uses:

- relation between pulsation and wave vector, or frequency and wave number and the speed of light c for light waves

$$c = \frac{\omega}{|\vec{k}|} = \lambda f$$

$$f = \frac{\omega}{2\pi} = \frac{c|\vec{k}|}{2\pi}$$

- Planck assumption that the minimum non-zero energy of a mode with frequency f is $E = hf$, and all the possible values of the energy of the mode is

$$E_m = mhf \quad , \quad m \in \mathbb{N} .$$

Taking a cubic box with sides $L_x = L_y = L_z = L$, the possible modes have (**todo** why? Which boundary condition? Periodic? Some physical? Just fictitious discretization?) in each direction wave-lengths $\lambda_n = \frac{L}{|\vec{n}|} = \frac{2\pi}{|\vec{k}|}$,

$$\vec{k} = \frac{2\pi}{L} \vec{n} .$$

Mode density in \vec{n} -domain is 2 mode per each volume of unit length (2 polarization), and thus the number of modes dN in an elementary volume is

$$dN = 2 d^3 \vec{n} ,$$

Changing variables, it's possible to find the mode density w.r.t. wave vector \vec{k} ,

$$dN = 2 d^3 \vec{n} = 2 \frac{L^3}{(2\pi)^3} d^3 \vec{k} ,$$

or with its absolute value, exploiting the isotropy of the density function - and writing the elementary volume using "spherical coordinates" $d^3 \vec{k} = 4\pi |\vec{k}|^2 d|\vec{k}|$,

$$\begin{aligned} dN &= \frac{V}{(2\pi)^3} 8\pi |\vec{k}|^2 d|\vec{k}| = \\ &= \frac{V}{(2\pi)^3} 8\pi \frac{8\pi^3}{c^3} f^2 df = \\ &= V \frac{8\pi}{c^3} f^2 df =: V g(f) df . \end{aligned}$$

Average energy of a mode

Using Boltzmann distribution (**why?**) for the energy distribution in a single mode,

$$P(E_r) = \frac{e^{-\beta E_r}}{Z},$$

with $E_r = r h f$, and the partition function

$$Z = \sum_s e^{-\beta E_s} = \sum_s e^{-\beta h f s} = \frac{1}{1 - e^{-\beta h f}}.$$

The average energy of the mode reads

$$\begin{aligned} \langle E \rangle &= \sum_r E_r P(E_r) = \\ &= \sum_r r h f \frac{e^{-\beta h f r}}{Z} = \\ &= h f (1 - e^{-\beta h f}) \sum_r r e^{-\beta h f r} = \\ &= h f (1 - e^{-\beta h f}) \frac{e^{-\beta h f}}{(1 - e^{-\beta h f})^2} = \\ &= \frac{h f}{e^{\beta h f} - 1}. \end{aligned}$$

Putting together the mode number density and the average energy of a mode, the energy density per unit volume, per frequency reads

$$\begin{aligned} u(f, T) &= \langle E \rangle(f) g(f) = \\ &= \frac{h f}{e^{\beta h f} - 1} \frac{8\pi}{c^3} f^2 = \\ &= \frac{8\pi h f^3}{c^3} \frac{1}{e^{\beta h f} - 1}. \end{aligned}$$

Property of the series

$$\sum_{n=0}^{+\infty} n x^n = \frac{x}{(1-x)^2}$$

Proof. If the series is convergent (is this the required condition?)

$$\frac{d}{dx} \sum_{n=0}^{+\infty} x^n = \frac{d}{dx} \frac{1}{1-x} = \frac{1}{(1-x)^2}$$

$$\frac{d}{dx} \sum_{n=0}^{+\infty} x^n = \sum_{n=0}^{+\infty} n x^{n-1}$$

$$x \frac{d}{dx} \sum_{n=0}^{+\infty} x^n = \sum_{n=0}^{+\infty} n x^n = \frac{x}{(1-x)^2}$$

Spectral radiance, B_f , so that an infinitesimal amount of power radiated by a surface ... is $dP = B_f(f, T) \cos \theta dA d\Omega df$

$$B_f(f, T) = \frac{2 h f^3}{c^2} \frac{1}{e^{\frac{h f}{k_B T}} - 1}.$$

This expression is obtained^[^nano-hub] assuming homogeneous radiation from a small hole cut into a wall of the box. Only half of the energy radiates through the hole - so factor $\frac{1}{2}$ in front of the energy density - through a solid angle 2π - and thus this process give the same result as a radiation of all the energy density in all the space directions, just providing the same factor $\frac{1}{4\pi}$. The flux of energy “has velocity” c and thus

$$B_f(f, T) = \frac{1}{4\pi} u_f(f, T) c .$$

Wien’s law. Wien’s law tells that the frequency f^* corresponding to the maximum of the spectral radiance of a black-body radiation described by Planck’s law is proportional to its temperature.

From direct evaluation of the derivative of the spectral radiance as a function of f ,

$$\begin{aligned} \partial_f B_f(f, T) &= \frac{2h}{c^2} \left[3f^2 \frac{1}{e^{\frac{hf}{k_B T}} - 1} + f^3 \left(-\frac{\frac{h}{k_B T} e^{\frac{hf}{k_B T}}}{\left(e^{\frac{hf}{k_B T}} - 1 \right)^2} \right) \right] = \\ &= \frac{2hf^2 e^{\frac{hf}{k_B T}}}{c^2 \left(e^{\frac{hf}{k_B T}} - 1 \right)^2} \left[3 \left(1 - e^{-\frac{hf}{k_B T}} \right) - \frac{hf}{k_B T} \right] . \end{aligned}$$

Now, if $\partial_f B_f(f, T) = 0$ the frequency is either $f = 0$, or the solution of the nonlinear algebraic equation

$$0 = 3 \left(1 - e^{-\frac{hf}{k_B T}} \right) - \frac{hf}{k_B T} .$$

Defining $x := \frac{hf}{k_B T}$, this equation becomes

$$0 = 3(1 - e^x) - x ,$$

whose solution $x^* \approx 2.82$ can be easily evaluated with an iterative method (or expressed in term of the Lambert’s function W , so loved at Stanford and on Youtube: they’d probaly like to look at tabulated values, or pose). Once the solution x^* of this non-dimensional equation is found, the frequency where maximum energy density occurs reads

$$f^* = \frac{k_B T}{h} x^* \simeq 2.82 \frac{k_B T}{h} .$$

Stefan-Boltzmann law.

$$\begin{aligned} \frac{P}{A} &= \int B_f(f, T) \cos \phi \, df \, d\Omega = \\ &= \int_{f=0}^{+\infty} \int_{\phi=0}^{\frac{\pi}{2}} \int_{\theta=0}^{2\pi} B_f(f, T) \cos \phi \sin \phi \, df \, d\phi \, d\theta = \\ &= \pi \int_{f=0}^{+\infty} B_f(f, T) \, df = \\ &= \frac{2\pi h}{c^2} \int_{f=0}^{+\infty} \frac{f^3}{e^{\frac{hf}{k_B T}} - 1} \, df = \\ &= \frac{2\pi h}{c^2} \left(\frac{k_B T}{h} \right)^4 \int_{u=0}^{+\infty} \frac{u^3}{e^u - 1} \, du . \end{aligned}$$

The value of the integral is $\frac{\pi^4}{15}$ and thus

$$\frac{P}{A} = \sigma T^4 \quad , \quad \sigma = \frac{2\pi^5 k_B^4}{15c^2 h^3} .$$

Example 2 (Energy density and radiance)

Radiance. The radiance $L_{e,\Omega}$ of a surface is the flux of energy per unit solid angle, per unit projected area of the source.

Spectral radiance in frequency is the radiance per unit frequency, $L_{e,\Omega,f} = \frac{\partial L_{e,\Omega}}{\partial f}$.

6.5.3 Fermi-Dirac

Statistics of undistinguishable components that can't be in the same (sub)level, obeying to the Pauli exclusion principle. Given the number of elementary components $\sum_i N_i = N$ and the energy $\sum_i N_i E_i = E$,

$$W_{FD,i} = \frac{G_i!}{(G_i - N_i)!N_i!} \quad , \quad W_{FD} = \prod_i W_{FD,i} . \quad (6.2)$$

Counting microstates

todo write page *Combinatorics* and add link

Most likely microstate. The approximate occupation number of the i^{th} level of the most likely microstate is

$$n_i := \frac{N_i}{G_i} = \frac{1}{1 + e^{\alpha + \beta E_i}} .$$

Optimization

$$\begin{aligned} J(N_i, \alpha, \beta) &= \ln W_{FD} + \alpha \left(N - \sum_i N_i \right) + \beta \left(E - \sum_i N_i E_i \right) = \\ &= \sum_i \{ \ln G_i! - \ln(G_i - N_i)! - \ln N_i! \} + \alpha \left(N - \sum_i N_i \right) + \beta \left(E - \sum_i N_i E_i \right) = \\ &= \sum_i \{ G_i \ln G_i - (G_i - N_i) \ln(G_i - N_i) - N_i \ln N_i \} + \alpha \left(N - \sum_i N_i \right) + \beta \left(E - \sum_i N_i E_i \right) = \end{aligned}$$

Using $\partial_n (n + a) \ln(n + a) = \ln(n + a) + 1$,

$$0 = \partial_{N_k} J \simeq \{ \ln(G_k - N_k) - \ln N_k \} - \alpha - \beta E_k ,$$

and thus

$$\begin{aligned} \ln \frac{G_k - N_k}{N_k} &= \alpha + \beta E_k , \\ \frac{G_k}{N_k} - 1 &= e^{\alpha + \beta E_k} \end{aligned}$$

The occupation number of the k level is

$$N_k = \frac{G_k}{1 + e^{\alpha + \beta E_k}} .$$

The average occupation of the G_k sublevels of the k level is

$$n_k := \frac{N_k}{G_k} = \frac{1}{1 + e^{\alpha + \beta E_k}} .$$

Meaning of α, β

STATISTICAL PHYSICS - STATISTICS MISCELLANEA

Information content and Entropy

Given a discrete random variable X with probability mass function $p_X(x)$, the self-information (**todo** *what about mutual information of random variables?*) is defined as the opposite of the logarithm of the mass function $p_X(x)$,

$$I_X(x) := -\ln(p_X(x)) .$$

Information content of independent random variables is additive. Since $p_{X,Y}(x,y) = p_X(x)p_Y(y)$,

$$I_{X,Y}(x,y) = -\ln(p_{X,Y}(x,y)) = -\ln(p_X(x)p_Y(y)) = -\ln p_X(x) - \ln p_Y(y) .$$

Shannon entropy. Shannon entropy of a discrete random variable X is defined as the expected value of the information content,

$$H(X) := \mathbb{E}[I_X(X)] = \sum p_X(x) I_X(x) = -\sum p_X \ln p_X(x) .$$

Gibbs entropy. Gibbs entropy was defined by J.W.Gibbs in 1878,

$$S = -k_B \sum_i p_i \ln p_i .$$

Additivity holds for independent random variables.

Boltzmann entropy. Boltzmann entropy holds for uniform distributions over Ω possible states, $p_i = \frac{1}{\Omega}$. Gibbs' entropy of this uniform distribution becomes

$$S = -k_B \Omega \frac{1}{\Omega} \ln \frac{1}{\Omega} = k_B \ln \Omega .$$

Entropy in Quantum Mechanics. todo

Boltzmann distribution

Given a set of discrete states with probability p_i , and the average measure as “macroscopic quantity” $E = \sum_i p_i E_i$, Boltzmann distribution maximizes the entropy (**todo** *Link to min info, max uncertainty*)

$$S = -k_B \sum_i p_i \ln p_i .$$

The distribution follows from the constrained optimization

$$\tilde{S} = S - \alpha \left(\sum_i p_i - 1 \right) - \beta \left(\sum_i p_i E_i - E \right)$$

$$0 = \partial_\alpha \tilde{S} = - \sum_i p_i - 1$$

$$0 = \partial_\beta \tilde{S} = - \sum_i p_i E_i - E$$

$$0 = \partial_{p_k} \tilde{S} = -k_B (\ln p_k + 1) - \alpha - \beta E_k$$

and thus

$$p_k = e^{-1 - \frac{\alpha}{k_B} - \frac{\beta}{k_B} E_k} = e^{-\left(1 + \frac{\alpha}{k_B}\right)} e^{-\frac{\beta}{k_B} E_k} = C e^{-\frac{\beta}{k_B} E_k},$$

and the normalization constant C is determined by normalization condition

$$1 = \sum_k p_k = C \sum_k e^{-\frac{\beta E_k}{k_B}}$$

The inverse $Z = C^{-1}$ is defined as the **partition function**,

$$Z = C^{-1} = \sum_k e^{-\frac{\beta E_k}{k_B}},$$

and the probability distribution becomes

$$p_k = \frac{e^{-\frac{\beta E_k}{k_B}}}{Z} = \frac{e^{-\frac{\beta E_k}{k_B}}}{\sum_i e^{-\frac{\beta E_i}{k_B}}}.$$

Properties.

$$\frac{p_k}{p_i} = e^{-\frac{\beta}{k_B} (E_k - E_i)}.$$

Thermodynamics. Comparison of statistics and classical thermodynamics

First principle of classical thermodynamics (for a monocomponent gas with no electric charge,...) reads

$$T dS = dE + P dV$$

Entropy for Boltzmann distribution reads

$$\begin{aligned} S &= -k_B \sum_i p_i \ln p_i = \\ &= -k_B \sum_i \left[p_i \left(-\frac{\beta E_i}{k_B} - \ln Z \right) \right] = \\ &= \beta \langle E \rangle + k_B \ln Z \\ \frac{1}{T} &= \left(\frac{\partial S}{\partial E} \right) \Big|_x = \\ &= \frac{\partial \beta}{\partial E} E + \beta + k_B \frac{\partial \ln Z}{\partial E} = \end{aligned}$$

todo

- write the derivative above clearly in terms of composite functions
- microscopical/statistical approach to the first principle of thermodynamics

Part IV

Quantum Mechanics

QUANTUM MECHANICS

- Principles and postulates
 - statistics and measurements outcomes (Heisenberg built its matrix mechanics only on observables...)
 - CCR
- angular momentum, spin, and atom

8.1 Mathematical tools for quantum mechanics

Definition 1 (Operator)

Definition 2 (Adjoint operator)

Given an operator $\hat{A} : U \rightarrow V$, its self-adjoint $\hat{A}^* : V \rightarrow U$ is the operator s.t.

$$(\mathbf{v}, \hat{A}\mathbf{u})_V = (\mathbf{u}, \hat{A}^*\mathbf{v})_U$$

holds for $\forall \mathbf{u} \in U, \mathbf{v} \in V$.

Definition 3 (Hermitian (self-adjoint) operator)

If $\hat{A} : U \rightarrow U$, it is a self-adjoint operator if $\hat{A}^* = \hat{A}$.

Self-adjoint operators have real eigenvalues, and orthogonal eigenvectors (at least those associated to different eigenvalues; those associated with the same eigenvalues can be used to build an orthogonal set of vectors with orthogonalization process).

8.2 Postulates of Quantum Mechanics

- ...
- Canonical Commutation Relation (CCR) and Canonical Anti-Commutation Relation...
- ...

8.3 Non-relativistic Mechanics

8.3.1 Statistical Interpretation and Measurement

Wave function

The state of a system is described by a wave function $|\Psi\rangle$

todo

- properties: domain, image,...
- unitary $1 = \langle\Psi|\Psi\rangle = |\Psi|^2$, for statistical interpretation of $|\Psi|^2$ as a density probability function

Operators and Observables

Physical **observable** quantities are represented by *Hermitian operators*. Possible outcomes of measurement are the eigenvalues of the operator

Given \hat{A} and the set of its eigenvectors $\{|A_i\rangle\}_i$ (**todo** continuous or discrete spectrum..., need to treat this difference quite in details), with associated eigenvalues $\{a_i\}_i$

$$\hat{A}|A_i\rangle = a_i|A_i\rangle$$

$$|\Psi\rangle = |A_i\rangle\langle A_i|\Psi\rangle = |A_i\rangle\Psi_i^A$$

$$\langle A_j|\Psi\rangle = \langle A_j|A_i\rangle\langle A_i|\Psi\rangle = \Psi_j^A$$

and thus

$$\Psi_j^A = \langle A_j|\Psi\rangle$$

$$\Psi_j^{A*} = \langle\Psi|A_j\rangle$$

- identity operator $\sum_i |A_i\rangle\langle A_i| = \mathbb{I}$, since

$$\sum_i |A_i\rangle\langle A_i|\Psi\rangle = \sum_i |A_i\rangle\langle A_i|\Psi_j^A A_j\rangle = \sum_i |A_i\rangle\delta_{ij}\Psi_j^A = \sum_i |A_i\rangle\Psi_i^A = |\Psi\rangle$$

- Normalization:

$$1 = \langle\Psi|\Psi\rangle = \Psi_j^{A*} \underbrace{\langle A_j|A_i\rangle}_{\delta_{ij}} \Psi_i^A = \sum_i |\Psi_i^A|^2$$

with $|\Psi_i^A|^2$ that can be interpreted as the probability of finding the system in state $|A_i\rangle$

- Expected value of the physical quantity in the a state $|\Psi\rangle$, with possible values a_i with probability $|\Psi_i^A|^2$

$$\begin{aligned}
 \bar{A}_\Psi &= \sum_i a_i |\Psi_i^A|^2 = \\
 &= \sum_i a_i \Psi_i^{A*} \Psi_i^A = \\
 &= \sum_i a_i \langle \Psi | A_i \rangle \langle A_i | \Psi \rangle = \\
 &= \langle \Psi | \left(\sum_i a_i |A_i\rangle \langle A_i| \right) | \Psi \rangle = \\
 &= \langle \Psi | \hat{A} | \Psi \rangle =
 \end{aligned}$$

since an operator \hat{A} can be written as a function of its eigenvalues and eigenvectors

$$\begin{aligned}
 \left(\sum_i a_i |A_i\rangle \langle A_i| \right) \Psi &= \left(\sum_i a_i |A_i\rangle \langle A_i| \right) c_k |A_k\rangle = \\
 &= \sum_i a_i |A_i\rangle c_i = \\
 &= \sum_i \hat{A} |A_i\rangle c_i = \\
 &= \hat{A} \sum_i |A_i\rangle c_i = \hat{A} |\Psi\rangle .
 \end{aligned}$$

Space Representation

Position operator $\hat{\mathbf{r}}$ has eigenvalues \mathbf{r} identifying the possible measurements of the position

$$\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle ,$$

being \mathbf{r} the result of the measurement (position in space, mathematically it could be a vector), and $|\mathbf{r}\rangle$ the state function corresponding to the measurement \mathbf{r} of the position.

- Result of measurement, \mathbf{r} , is a position in space. As an example, it could be a point in an Euclidean space $P \in E^n$. It could be written using properties of Dirac's delta "function"

$$\mathbf{r} = \int_{\mathbf{r}'} \delta(\mathbf{r}' - \mathbf{r}) \mathbf{r}' d\mathbf{r}'$$

- Projection of wave function over eigenstates of position operator

$$\begin{aligned}
 \langle \mathbf{r} | \Psi \rangle(t) &= \Psi(\mathbf{r}, t) = \int_{\mathbf{r}'} \delta(\mathbf{r} - \mathbf{r}') \Psi(\mathbf{r}', t) d\mathbf{r}' = \\
 &= \int_{\mathbf{r}'} \langle \mathbf{r} | \mathbf{r}' \rangle \Psi(\mathbf{r}', t) d\mathbf{r}' = \\
 &= \int_{\mathbf{r}'} \langle \mathbf{r} | \mathbf{r}' \rangle \langle \mathbf{r}' | \Psi \rangle(t) d\mathbf{r}' = \\
 &= \langle \mathbf{r} | \underbrace{\left(\int_{\mathbf{r}'} |\mathbf{r}'\rangle \langle \mathbf{r}'| d\mathbf{r}' \right)}_{=\hat{\mathbf{I}}} | \Psi \rangle(t) .
 \end{aligned}$$

- having used orthogonality (**todo** why? provide definition and examples of operators with continuous spectrum)

$$\langle \mathbf{r}' | \mathbf{r} \rangle = \delta(\mathbf{r}' - \mathbf{r})$$

- Expansion of a state function $|\Psi\rangle(t)$ over the basis of the position operator

$$|\Psi\rangle(t) = \hat{\mathbf{1}}|\Psi\rangle(t) = \left(\int_{\mathbf{r}'} |\mathbf{r}'\rangle \langle \mathbf{r}'| d\mathbf{r}' \right) |\Psi\rangle(t) = \int_{\mathbf{r}'} |\mathbf{r}'\rangle \langle \mathbf{r}'|\Psi\rangle(t) d\mathbf{r}' .$$

- Unitarity and probability density

$$\begin{aligned} 1 &= \langle \Psi|\Psi\rangle(t) = \langle \Psi| \left(\int_{\mathbf{r}'} |\mathbf{r}'\rangle \langle \mathbf{r}'| d\mathbf{r}' \right) |\Psi\rangle \\ &= \int_{\mathbf{r}'} \langle \Psi|\mathbf{r}'\rangle \langle \mathbf{r}'|\Psi\rangle d\mathbf{r}' \\ &= \int_{\mathbf{r}'} \Psi^*(\mathbf{r}', t) \Psi(\mathbf{r}', t) d\mathbf{r}' \\ &= \int_{\mathbf{r}'} |\Psi(\mathbf{r}', t)|^2 d\mathbf{r}' \end{aligned}$$

and thus $|\Psi(\mathbf{r}, t)|^2$ can be interpreted as the **probability density function** of measuring position of the system equal to \mathbf{r}' .

- Average value of the operator

$$\begin{aligned} \bar{\mathbf{r}} &= \langle \Psi|\hat{\mathbf{r}}|\Psi\rangle = \\ &= \int_{\mathbf{r}'} \langle \Psi|\mathbf{r}'\rangle \langle \mathbf{r}'|\hat{\mathbf{r}}| \int_{\mathbf{r}''} |\mathbf{r}''\rangle \langle \mathbf{r}''|\Psi\rangle d\mathbf{r}'' \\ &= \int_{\mathbf{r}'} \int_{\mathbf{r}''} \langle \Psi|\mathbf{r}'\rangle \langle \mathbf{r}'|\hat{\mathbf{r}}|\mathbf{r}''\rangle \langle \mathbf{r}''|\Psi\rangle d\mathbf{r}' d\mathbf{r}'' = \\ &= \int_{\mathbf{r}'} \int_{\mathbf{r}''} \langle \Psi|\mathbf{r}'\rangle \underbrace{\langle \mathbf{r}'|\mathbf{r}''\rangle}_{=\delta(\mathbf{r}'-\mathbf{r}'')} \mathbf{r}'' \langle \mathbf{r}''|\Psi\rangle d\mathbf{r}' d\mathbf{r}'' = \\ &= \int_{\mathbf{r}'} \langle \Psi|\mathbf{r}'\rangle \mathbf{r}' \langle \mathbf{r}'|\Psi\rangle d\mathbf{r}' = \\ &= \int_{\mathbf{r}'} \Psi^*(\mathbf{r}', t) \mathbf{r}' \Psi(\mathbf{r}', t) d\mathbf{r}' = \\ &= \int_{\mathbf{r}'} |\Psi(\mathbf{r}', t)|^2 \mathbf{r}' d\mathbf{r}' . \end{aligned}$$

Momentum Representation

Momentum operator as the limit of ... **todo** prove the expression of the momentum operator as the limit of the generator of translation

$$\langle \mathbf{r}|\hat{\mathbf{p}} = -i\hbar \nabla \langle \mathbf{r}|$$

- Spectrum

$$\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle$$

$$\langle \mathbf{r}|\hat{\mathbf{p}}|\mathbf{p}\rangle = -i\hbar \nabla \langle \mathbf{r}|\mathbf{p}\rangle = \mathbf{p} \langle \mathbf{r}|\mathbf{p}\rangle$$

and thus the eigenvectors in space base $\mathbf{p}(\mathbf{r}) = \langle \mathbf{r}|\mathbf{p}\rangle$ are the solution of the differential equation

$$-i\hbar \nabla \mathbf{p}(\mathbf{r}) = \mathbf{p} \mathbf{p}(\mathbf{r}) ,$$

that in Cartesian coordinates reads

$$-i\hbar\partial_j p_k(\mathbf{r}) = p_j p_k(\mathbf{r})$$

$$p_k(\mathbf{r}) = p_{k,0} \exp\left[i\frac{p_j}{\hbar}r_j\right]$$

or

$$\langle \mathbf{r} | \mathbf{p} \rangle = \mathbf{p}(\mathbf{r}) = \mathbf{p}_0 \exp\left[i\frac{\mathbf{p} \cdot \mathbf{r}}{\hbar}\right]$$

todo

- normalization factor $\frac{1}{(2\pi)^{\frac{3}{2}}}$

$$\mathcal{F}\{\delta(x)\}(k) = \int_{-\infty}^{\infty} \delta(x) e^{-ikx} dx = 1$$

- Fourier transform and inverse Fourier transform: definitions and proofs (link to a math section)
- representation in basis of wave vector operator $\hat{\mathbf{k}}, \hat{\mathbf{p}} = \hbar\hat{\mathbf{k}}$

From position to momentum representation

Momentum and wave vector, $\mathbf{p} = \hbar\mathbf{k}$

$$\begin{aligned} \langle \mathbf{p} | \Psi \rangle &= \langle \mathbf{p} | \int_{\mathbf{r}'} |\mathbf{r}'\rangle \langle \mathbf{r}' | \Psi \rangle d\mathbf{r}' = \\ &= \int_{\mathbf{r}'} \langle \mathbf{p} | \mathbf{r}' \rangle \langle \mathbf{r}' | \Psi \rangle d\mathbf{r}' = \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{r}'} \exp\left[i\frac{\mathbf{p} \cdot \mathbf{r}'}{\hbar}\right] \langle \mathbf{r}' | \Psi \rangle d\mathbf{r}' = \end{aligned}$$

Relation between position and wave-number representation can be represented with a Fourier transform

$$\begin{aligned} \langle \mathbf{k} | \Psi \rangle &= \langle \mathbf{k} | \int_{\mathbf{r}'} |\mathbf{r}'\rangle \langle \mathbf{r}' | \Psi \rangle d\mathbf{r}' = \\ &= \int_{\mathbf{r}'} \langle \mathbf{k} | \mathbf{r}' \rangle \langle \mathbf{r}' | \Psi \rangle d\mathbf{r}' = \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{r}'} \exp[i\mathbf{k} \cdot \mathbf{r}'] \langle \mathbf{r}' | \Psi \rangle d\mathbf{r}' = \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{r}'} \exp[i\mathbf{k} \cdot \mathbf{r}'] \Psi(\mathbf{r}') d\mathbf{r}' = \\ &= \mathcal{F}\{\Psi(\mathbf{r})\}(\mathbf{k}) \end{aligned}$$

8.3.2 Schrodinger Equation

$$i\hbar \frac{d}{dt} |\Psi\rangle = \hat{H} |\Psi\rangle$$

being \hat{H} the Hamiltonian operator and $|\Psi\rangle$ the wave function, as a function of time t as an independent variable.

Stationary States

Eigenspace of the Hamiltonian operator

$$\hat{H}|\Psi_k\rangle = E_k|\Psi_k\rangle,$$

with E_k possible values of energy measurements. *If no eigenstates with the same eigenvalue exists, then...otherwise... Without external influence **todo** be more detailed!*, energy values and eigenstates of the systems are constant in time.

Thus, expanding the state of the system $|\Psi\rangle$ over the stationary states gives $|\Psi_k\rangle$, $|\Psi\rangle = |\Psi_k\rangle c_k(t)$, and inserting in Schrodinger equation

$$i\hbar\dot{c}_k|\Psi_k\rangle = c_k E_k |\Psi_k\rangle$$

and exploiting orthogonality of eigenstates, a diagonal system for the amplitudes of stationary states arises,

$$i\hbar\dot{c}_k = c_k E_k.$$

whose solution reads

$$c_k(t) = c_{k,0} \exp\left[-i\frac{E_k}{\hbar}t\right]$$

Thus the state of the system evolves like a superposition of monochromatic waves with frequencies $\omega_k = \frac{E_k}{\hbar}$,

$$|\Psi\rangle = |\Psi_k\rangle c_k(t) = |\Psi_k\rangle c_{k,0} \exp\left[-i\frac{E_k}{\hbar}t\right].$$

$$\begin{aligned} \frac{d}{dt}\bar{A} &= \frac{d}{dt}(\langle\Psi|\hat{A}|\Psi\rangle) = \\ &= \frac{d}{dt}\langle\Psi|\hat{A}|\Psi\rangle + \langle\Psi|\frac{d\hat{A}}{dt}|\Psi\rangle + \langle\Psi|\hat{A}\frac{d}{dt}|\Psi\rangle = \\ &= \langle\Psi|\frac{d\hat{A}}{dt}|\Psi\rangle + \frac{i}{\hbar}\langle\Psi|\hat{H}\hat{A}|\Psi\rangle - \frac{i}{\hbar}\langle\Psi|\hat{A}\hat{H}|\Psi\rangle = \\ &= \langle\Psi|\left(\frac{i}{\hbar}[\hat{H}, \hat{A}] + \frac{d\hat{A}}{dt}\right)|\Psi\rangle. \end{aligned}$$

Pictures

- Schrodinger
- Heisenberg
- Interaction

Schrodinger

If \hat{H} not function of time

$$|\Psi\rangle(t) = \exp\left[-i\frac{\hat{H}}{\hbar}(t-t_0)\right]|\Psi\rangle(t_0) = \hat{U}(t, t_0)|\Psi\rangle(t_0)$$

$$\bar{A} = \langle\Psi|\hat{A}|\Psi\rangle = \langle\Psi_0|\hat{U}^*(t, t_0)\hat{A}\hat{U}(t, t_0)|\Psi_0\rangle$$

Heisenberg

...

for \hat{H} independent from time t ,

$$\begin{aligned}\frac{d}{dt}\hat{\mathbf{r}} &= \frac{i}{\hbar} [\hat{H}, \hat{\mathbf{r}}] \\ \frac{d}{dt}\hat{\mathbf{p}} &= \frac{i}{\hbar} [\hat{H}, \hat{\mathbf{p}}]\end{aligned}$$

Hamiltonian Mechanics

From Lagrange equations

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = Q_q$$

q generalized coordinates, $p := \frac{\partial L}{\partial \dot{q}}$ generalized momenta.

Hamiltonian

$$H(p, q, t) = p\dot{q} - L(\dot{q}, q, t)$$

Increment of the Hamiltonian

$$\begin{aligned}dH &= \partial_p H dp + \partial_q H dq + \partial_t H dt \\ dH &= \dot{q} dp + p d\dot{q} - \partial_{\dot{q}} L d\dot{q} - \partial_q L dq - \partial_t L dt = \\ &= \dot{q} dp - \partial_q L dq - \partial_t L dt = \\ &= \dot{q} dp - (\dot{p} + Q_q) dq - \partial_t L dt = \\ &\quad \begin{cases} \frac{\partial H}{\partial p} = \dot{q} \\ \frac{\partial H}{\partial q} = -\frac{\partial L}{\partial q} = -\dot{p} + Q_q \\ \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} \end{cases}\end{aligned}$$

Physical quantity $f(p(t), q(t), t)$. Its time derivative reads

$$\begin{aligned}\frac{df}{dt} &= \frac{\partial f}{\partial p} \dot{p} + \frac{\partial f}{\partial q} \dot{q} + \frac{\partial f}{\partial t} = \\ &= \frac{\partial f}{\partial p} \left[-\frac{\partial H}{\partial q} + Q_q \right] + \frac{\partial f}{\partial q} \frac{\partial H}{\partial p} + \frac{\partial f}{\partial t} = \\ &= \{H, f\} + \partial_t f + Q_q \partial_p f\end{aligned}$$

If $Q_q = 0$, the correspondence between quantum mechanics and classical mechanics

$$\begin{aligned}\frac{df}{dt} = \{H, f\} + \partial_t f &\quad \leftrightarrow \quad \frac{d}{dt} \overline{\hat{f}} = \frac{i}{\hbar} [\hat{H}, \hat{f}] + \overline{\frac{\partial \hat{f}}{\partial t}} \\ \{H, f\} &\quad \leftrightarrow \quad \frac{i}{\hbar} [\hat{H}, \hat{f}]\end{aligned}$$

Interaction

8.3.3 Matrix Mechanics

Attualization of 1925 papers

...to find the canonical commutation relation,

$$[\hat{\mathbf{r}}, \hat{\mathbf{p}}] = i\hbar \mathbf{1}.$$

$$\begin{aligned} [\hat{\mathbf{r}}, \hat{\mathbf{p}}] &= \hat{\mathbf{r}}\hat{\mathbf{p}} - \hat{\mathbf{p}}\hat{\mathbf{r}} = \\ &= \hat{\mathbf{r}} \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| d\mathbf{r} \hat{\mathbf{p}} - \hat{\mathbf{p}} \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| d\mathbf{r} \hat{\mathbf{r}} \int_{\mathbf{r}'} |\mathbf{r}'\rangle \langle \mathbf{r}'| d\mathbf{r}' = \\ &= - \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| i\hbar \nabla \langle \mathbf{r}| d\mathbf{r} - \hat{\mathbf{p}} \int_{\mathbf{r}} \int_{\mathbf{r}'} |\mathbf{r}\rangle \langle \mathbf{r}| \underbrace{\langle \mathbf{r}|\mathbf{r}'\rangle}_{\delta(\mathbf{r}-\mathbf{r}')} \langle \mathbf{r}'| d\mathbf{r}' = \\ &= - \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| i\hbar \nabla \langle \mathbf{r}| d\mathbf{r} - \hat{\mathbf{p}} \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| d\mathbf{r} = \\ &= - \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| i\hbar \nabla \langle \mathbf{r}| d\mathbf{r} - \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| d\mathbf{r} \hat{\mathbf{p}} \int_{\mathbf{r}'} |\mathbf{r}'\rangle \langle \mathbf{r}'| d\mathbf{r}' = \\ &= - \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| i\hbar \nabla \langle \mathbf{r}| d\mathbf{r} + \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| i\hbar \nabla \langle \mathbf{r}| d\mathbf{r} \int_{\mathbf{r}'} |\mathbf{r}'\rangle \langle \mathbf{r}'| d\mathbf{r}' = \dots \\ [\hat{\mathbf{r}}, \hat{\mathbf{p}}] |\Psi\rangle &= - \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| i\hbar \nabla \Psi(\mathbf{r}, t) + \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| i\hbar \nabla (\mathbf{r} \Psi(\mathbf{r}, t)) = \\ &= - \int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| i\hbar [\mathbf{r} \nabla \Psi(\mathbf{r}, t) + \mathbf{1} \Psi(\mathbf{r}, t) + \mathbf{r} \nabla \Psi(\mathbf{r}, t)] = \\ &= i\hbar \underbrace{\int_{\mathbf{r}} |\mathbf{r}\rangle \langle \mathbf{r}| d\mathbf{r}}_{\mathbf{1}} |\Psi\rangle, \end{aligned}$$

and since $|\Psi\rangle$ is arbitrary

$$[\hat{\mathbf{r}}, \hat{\mathbf{p}}] = i\hbar \mathbf{1}.$$

$$[\hat{r}_a, \hat{p}_b] = i\hbar \delta_{ab}.$$

8.3.4 Heisenberg Uncertainty “principle”

- Heisenberg uncertainty “principle” is a relation between product of variance of two physical quantities and their commutation,
- **todo** relation with measurement process and outcomes. Commutation as a measurement process: first measure B and then A , or first measure A and then B

$$\sigma_A \sigma_B \geq \frac{1}{2} |\overline{[\hat{A}, \hat{B}]}|.$$

Proof of Heisenberg uncertainty “principle”

$$\begin{aligned}
 \sigma_A^2 \sigma_B^2 &= \langle \Psi | (\hat{A} - \bar{A})^2 | \Psi \rangle \langle \Psi | (\hat{B} - \bar{B})^2 | \Psi \rangle = \\
 &= \langle (\hat{A} - \bar{A})\Psi | (\hat{A} - \bar{A})\Psi \rangle \langle (\hat{B} - \bar{B})\Psi | (\hat{B} - \bar{B})\Psi \rangle = \\
 &= \|(\hat{A} - \bar{A})\Psi\|^2 \|(\hat{B} - \bar{B})\Psi\|^2 = \\
 &\geq \left| \langle (\hat{A} - \bar{A})\Psi | (\hat{B} - \bar{B})\Psi \rangle \right|^2 = \\
 &= \left| \langle \Psi | (\hat{A} - \bar{A})(\hat{B} - \bar{B})\Psi \rangle \right|^2 = \\
 &= \left| \langle \Psi | \hat{A}\hat{B} - \hat{A}\bar{B} - \bar{A}\hat{B} + \bar{A}\bar{B} | \Psi \rangle \right|^2 = \\
 &= \left| \langle \Psi | \hat{A}\hat{B} - \bar{A}\hat{B} | \Psi \rangle \right|^2 = \\
 &= \left| \frac{\langle \Psi | \hat{A}\hat{B} - \hat{B}\hat{A} | \Psi \rangle}{2i} \right|^2 = \\
 &= \frac{|\langle \Psi | [\hat{A}, \hat{B}] | \Psi \rangle|^2}{4} = \frac{1}{4} \left| \overline{[\hat{A}, \hat{B}]} \right|^2
 \end{aligned}$$

having used Cauchy triangle inequality and

$$|z| = \frac{\operatorname{re}\{z\} + \operatorname{re}\{z^*\}}{2} = \frac{\operatorname{im}\{z\} - \operatorname{im}\{z^*\}}{2i}$$

Heisenberg uncertainty principles applied to position and momentum reads

$$\sigma_{r_a} \sigma_{p_b} \geq \frac{1}{2} \left| \overline{[\hat{r}_a, \hat{p}_b]} \right| = \frac{\hbar}{2} \delta_{ab} .$$

8.4 Many-body problem

Wave function with symmetries: Fermions and Bosons

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