Week 7

Functions

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Ecole Polytechnique Fédérale de Lausanne

Overview

- Limits and Continuity
- Differentiability and Taylor Expansions

- Binary phase diagrams
- Lennard-Jones potential (also with Prof. Carter)

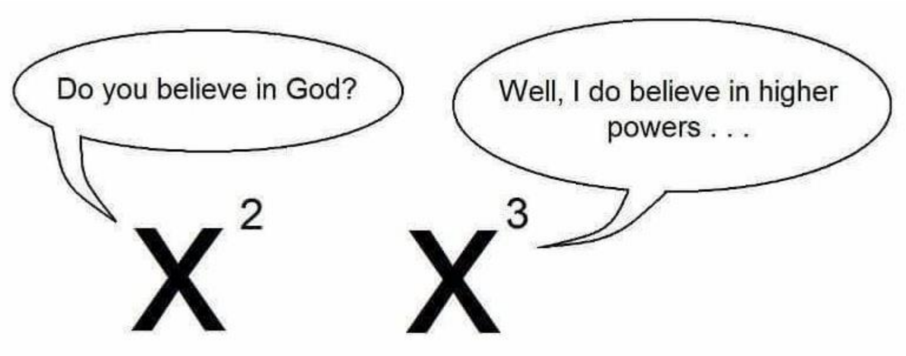
- Exam: Thursday 22nd January 2026 - 9h15 to 12h15 in ELD 020

The concept of functions

- The concept of Functions has been developed slowly over centuries of discoveries, and it is hard to bring forward one particular mathematician associated with it.

- In 1755, in his *Institutiones calculi differentialis,* Swiss mathematician Leonhard Euler gave a more general concept of a function that is very close to our modern understanding:

"When certain quantities depend on others in such a way that they undergo a change when the latter change, then the first are called *functions* of the second. This name has an extremely broad character; it encompasses all the ways in which one quantity can be determined in terms of others."



Leonhard Euler (1707-1783)

- Euler popularized the Greek letter **π** to denote the ratio of a circle's circumference to its diameter, was the first using the notation **f(x)** for the value of a function, the letter ***i*** to express the imaginary unit, the Greek letter **Σ** to express summations, the Greek letter **Δ** for finite differences. He gave the current definition of the constant ***e***, the base of the natural logarithm, now known as Euler's number.

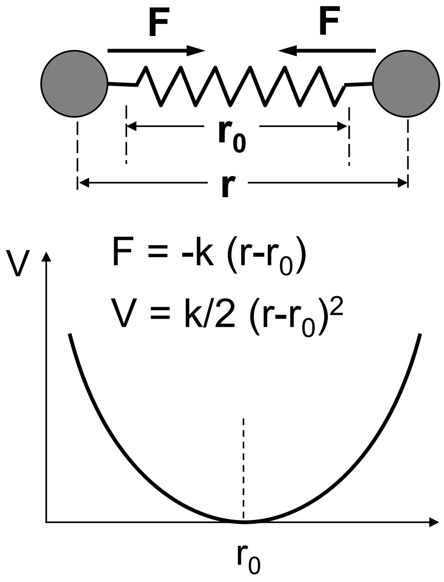
The concept of functions

- Given two sets of real numbers, a domain (often referred to as the x-values, and interval *I*) and a co-domain (often referred to as the y-values), a real function assigns to each x-value a *unique* y-value.

- *Injective function* (or injection): function *f* that maps distinct elements of its domain to distinct elements; that is, $f(x_1) = f(x_2)$ implies $x_1 = x_2$.

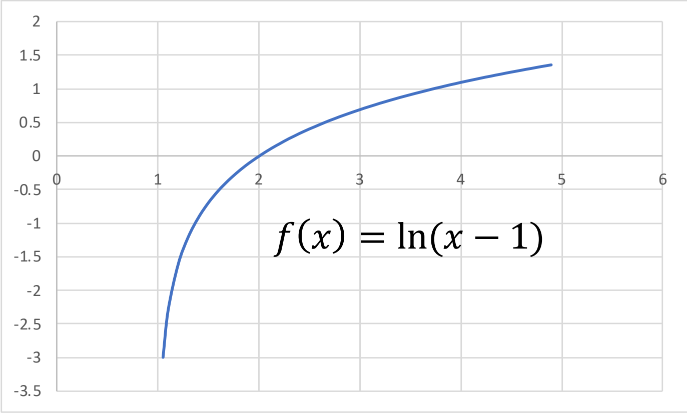
- *Surjective functions* (or surjection): a function *f* such that every element y can be mapped from element *x* so that $f(x) = y$.

- Example: the function $f(x) = x^2$ is injective and surjective (ie bijective) from $I = \mathbb{R}_+ \; to \; \mathbb{R}_+$. It is not injective from $I = \mathbb{R} \; to \; \mathbb{R}_+$, and not surjective $I = \mathbb{R} \; to \; \mathbb{R}_-$.



$$F = -k\,(r-r_0)$$

$$V = k/2\,(r-r_0)^2$$



$$f(x) = \ln(x-1)$$

- $f(x) = \ln(x-1)$ is not defined for $x \leq 1$. It is injective and surjective from $I =]1, +\infty[\; to \; \mathbb{R}$.

- The domains of definition are hence very important when defining the properties of functions : physically but also mathematically !

The concept of functions

- Functions defined on a domain, often a part $\mathrm{I} \subset \mathbb{R}$, form an associative and commutative $\mathbb{R}$-algebra (often denoted K^I) with the common addition, multiplication, and the product of a function with a scalar

$$\begin{cases} \forall f,g \in \mathbb{K}^X, \forall x \in X, & (f+g)(x) = f(x)+g(x) \\ \forall f,g \in \mathbb{K}^X, \forall x \in X, & (fg)(x) = f(x)g(x) \\ \forall \lambda \in \mathbb{K}, \forall f \in \mathbb{K}^X, \forall x \in X, & (\lambda f)(x) = \lambda f(x) \end{cases}.$$

- Other definitions:
  - Composition: if a function f is defined from I to X, and g is defined over X, then one can define the function $\forall x \in I,\ h(x) = gof(x)$.
  - f^{-1} is the inverse of f and is defined such that $f^{-1}of = fof^{-1} = I_d$ *(the identity function).*
  - A function is even (odd) *if* $\forall x \in I, f(x) = f(-x)$ $(f(x) = -f(-x))$
  - Periodicity: *f* is periodic of period *T* if $\forall x \in I, f(x+T) = f(x)$.

- Limits of real functions:

  - A function $f: I \to \mathbb{R}$ with *I* including $+\infty$, admits l for limit when x goes to infinity if and only if

$$\forall \varepsilon > 0, \exists A > 0, \forall x \in I, (x \geq A \Longrightarrow |f(x) - l| < \varepsilon)$$

  - A function $f: I \to \mathbb{R}$ with *I* including $+\infty$, admits $+\infty$ for limit when x goes to infinity if and only if

$$\forall A > 0, \exists A' > 0, \forall x \in I, (x \geq A' \Longrightarrow f(x) \geq A)$$

The important notion of limits

- Limits of functions **at finite values** are very important and can be defined by looking at the limit of sequences:

  - A function $f\colon I \to \mathbb{R}$ (or other domain) admits l for limit in a point $a \in I$ if and only if

  For all sequence $(u_n)_{n\in\mathbb{N}}$ such that $\lim\limits_{n\to\infty} u_n = a$, $\lim\limits_{n\to\infty} f(u_n) = l$.

  - One can express this without sequences:

$$\forall \varepsilon > 0, \exists \alpha > 0, \forall x \in I, |x - a| < \alpha \Longrightarrow |f(x) - l| < \varepsilon$$

  - Functions can diverge to $\pm\infty$ at finite values of the argument:

  Divergence to $+\infty$: $\forall A > 0, \exists \alpha > 0, \forall x \in I, |x - a| < \alpha \Longrightarrow f(x) \geq A$
  Divergence to $-\infty$: $\forall B < 0, \exists \alpha > 0, \forall x \in I, |x - a| < \alpha \Longrightarrow f(x) \leq B$

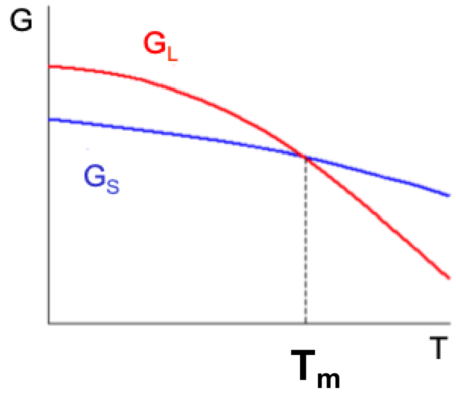
- Like for Sequences:
  - If f is increasing (decreasing) and has an upper bound (lower bound), then it converges.

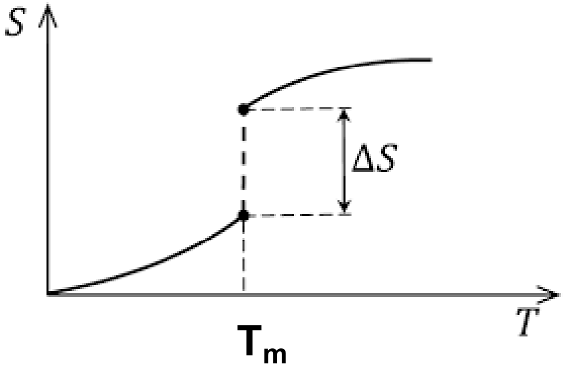
  - If f is increasing (decreasing) and has no upper bound (lower bound), then it tends to $+\infty$ $(-\infty)$.

Right and Left limits

- The concepts of limits and continuity of functions are essential in Materials Science.
- To apprehend it, it is essential to distinguish the limit when we approach a real number *l* from a sequence greater or smaller than *l.*

First order phase transition for a pure material (unitary)





At constant pressure:

$$G_S(Tm) = G_L(Tm)$$

$$\Delta S = \frac{\Delta H(T_m)}{T_m}$$

- $f: I \to \mathbb{R}$ (or other domain) admits a right limit l at a point $a \in I$ if and only if
For all sequence $(u_n)_{n\in\mathbb{N}}$ such that $\lim_{n\to\infty} u_n = a$ and $\forall n \in \mathbb{N}\ u_n > a$, $\lim_{n\to\infty} f(u_n) = l$.

One can express this without sequences:

$f: I \to \mathbb{R}$ has a right limit l at $a \in I$ if:

$\forall \varepsilon > 0, \exists \alpha > 0, \forall x \in I, 0 < x - a \le \alpha \Longrightarrow |f(x) - l| < \varepsilon$ Notation: $\lim_{x\to a^+} f(x) = l$

$f: I \to \mathbb{R}$ has a left limit l at $a \in I$ if:

$\forall \varepsilon > 0, \exists \alpha > 0, \forall x \in I, 0 < a - x \le \alpha \Longrightarrow |f(x) - l| < \varepsilon$ Notation: $\lim_{x\to a^-} f(x) = l$

Results of limits

- For $(\lambda, l, l') \in \mathbb{C}^3, f, g\colon I \to \mathbb{R}$ f,g admit l and l' as limit at a point $a \in I$ respectively:

$$f(x) \xrightarrow[x\to a]{} l \Longrightarrow |f(x)| \xrightarrow[x\to a]{} |l|$$

$$f(x) \xrightarrow[x\to a]{} 0 \Longleftrightarrow |f(x)| \xrightarrow[x\to a]{} 0$$

$$\left.\begin{array}{l} f(x) \xrightarrow[x\to a]{} l \\ g(x) \xrightarrow[x\to a]{} l' \end{array}\right\} \Longrightarrow f(x)+g(x) \xrightarrow[x\to a]{} l+l'$$

$$f(x) \xrightarrow[x\to a]{} l \Longrightarrow \lambda f(x) \xrightarrow[x\to a]{} \lambda l$$

$$\left\{\begin{array}{l} f(x) \xrightarrow[x\to a]{} 0 \\ g \quad \text{is bounded around a} \end{array}\right| \Longrightarrow f(x)g(x) \xrightarrow[x\to a]{} 0$$

$$\left.\begin{array}{l} f(x) \xrightarrow[x\to a]{} l \\ g(x) \xrightarrow[x\to a]{} l' \end{array}\right\} \Longrightarrow f(x)g(x) \xrightarrow[x\to a]{} ll'$$

$$\left.\begin{array}{l} g(x) \xrightarrow[x\to a]{} l' \\ l' \neq 0 \end{array}\right\} \Longrightarrow \frac{1}{g(x)} \xrightarrow[x\to a]{} \frac{1}{l'}$$

$$\left.\begin{array}{l} f(x) \xrightarrow[x\to a]{} l \\ g(x) \xrightarrow[x\to a]{} l' \\ l' \neq 0 \end{array}\right\} \Longrightarrow \frac{f(x)}{g(x)} \xrightarrow[x\to a]{} \frac{l}{l'}.$$

- If f is complex, then:

$$f : I \longrightarrow \mathbb{C},\ (\alpha, \beta) \in \mathbb{R}^2$$

$$f(x) \xrightarrow[x\to a]{} \alpha + \mathrm{i}\beta \Longleftrightarrow \left\{\begin{array}{l} (\text{Ré}\, f)(x) \xrightarrow[x\to a]{} \alpha \\ (\text{Im}\, f)(x) \xrightarrow[x\to a]{} \beta. \end{array}\right.$$

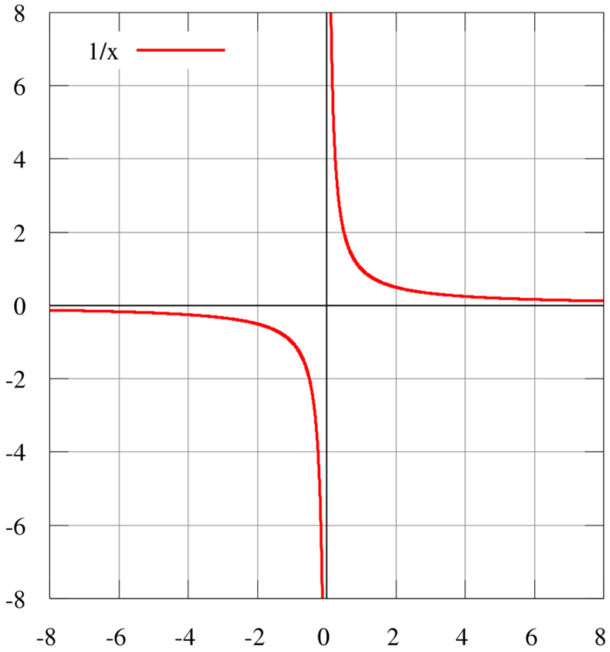
Continuous functions

- A function is continuous if arbitrarily small changes in its value can be assured by restricting to sufficiently small changes of its argument.

- A function $f: I \to \mathbb{R}$ with $I \subset \mathbb{R}$, f is continuous at the point $x_0 \in I$ if:

$$\forall \varepsilon > 0, \exists \alpha > 0, \forall x \in I, |x - x_0| < \alpha \Longrightarrow |f(x) - f(x_0)| < \varepsilon$$

It is equivalent to say that f is continuous at point $x_0 \in I$ if and only if **f has a right and left limit at x_0 and the limits are equal. (i.e. f must have $f(x_0)$ as a limit at x_0).**



Continuous functions

- Definition with sequences:

A function $f: I \to \mathbb{R}$ (or other domain) admits l for limit in a point $a \in I$ if and only if :

For all sequence $(u_n)_{n\in\mathbb{N}}$ such that $\lim\limits_{n\to\infty} u_n = a$, $\lim\limits_{n\to\infty} f(u_n) = f(a)$

- Important results
  - If *f* and *g* are two continuous functions over an interval I:
    - $|f|$ is continuous
    - $f + g$ is also continuous over I,
    - $\lambda f, \lambda \in \mathbb{R}\ or\ \mathbb{C}$, is continuous;
    - $f \times g$ is continuous;
    - If $g \neq 0$ over I, f/g is continuous;
    - **If $\boldsymbol{g}$ is continuous over $\boldsymbol{f(I)}$, $\boldsymbol{h(x) = gof(x)}$ is continuous.**
    - f^{-1}, if defined, is continuous over $f(I)$.
    - **If f is complex , it is continuous if and only if its real and imaginary parts are.**

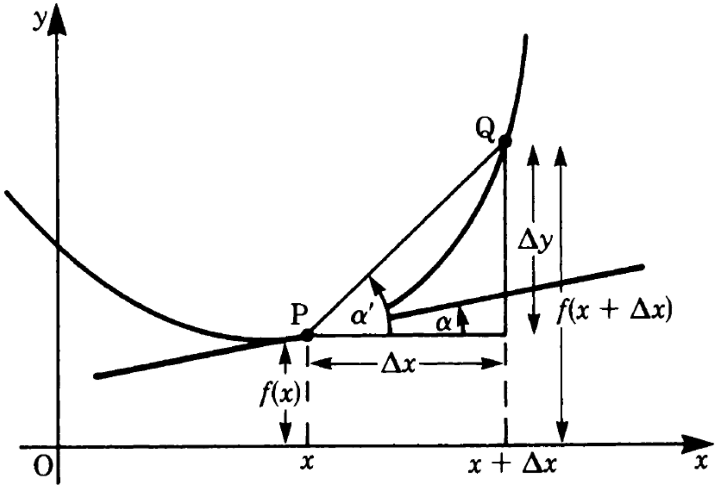
- **Extreme value theorem**:

If $f: \mathbb{R} \to \mathbb{R}$ is continuous over a segment $[a, b] \subset \mathbb{R}$, then there exist two real numbers c and d in [a, b] such that f(c) is the minimum and f(d) is the maximum value of f(x).
Or

$$\exists c, d \in [a, b], such\ that\ f(c) = inf_{[a,b]} f(x), and\ f(d) = sup_{[a,b]} f(x)$$

Differentiability

- What matters the most in the study of a function representing a physical model is its values at certain important input, but also how it varies as the input argument is changed.



- The variation of a curve can be locally approximated by the slope joining two points of the curve near-by.
- As the distance $\Delta x \to 0$, we approach the tangent of the function:

$$\tan\alpha = \lim_{\alpha' \to \alpha} \tan\alpha' = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

- If the difference quotient Δy/Δx has a limit as Δx → 0, this limit is called the derivative or differential coefficient of the function $y = f(x)$ with respect to x and we write:

$$y' = f'(x) = \frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x} f(x) = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

- More rigorously, a function $f\colon I \to \mathbb{R}$ with $I \subset \mathbb{R}$, is differentiable at $x \in I$ if:

$$\forall \varepsilon > 0, \exists \alpha > 0, \forall h \in I, |h| < \alpha \Longrightarrow \left| \frac{f(x+h) - f(x)}{h} - l \right| < \varepsilon$$

$$l = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} = f'(x)$$

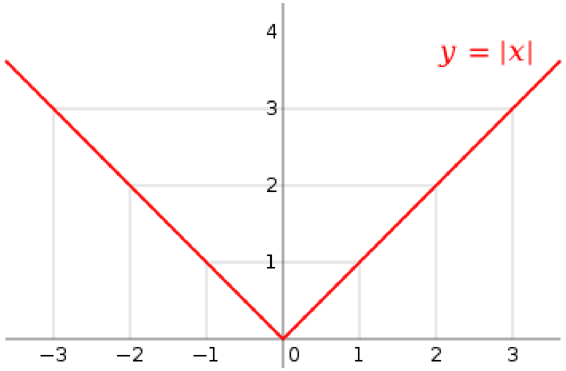
Differentiability

- A function f as defined earlier can be right and / or left differentiable if $\frac{f(x+h)-f(x)}{h}$ admits a right and left limit respectively.

- **Corollary**: f is differentiable at $a \in I$ if it is right and left differentiable, and the values are equal.

- **If a function is differentiable at point a, it is continuous at a.**

- The reverse is not true !



- Important immediate results:
  - f is increasing (decreasing) over a domain *I* if and only if $\forall x \in I, f'(x) > 0$ $(f'(x) < 0)$.

- If $f: \mathbb{R} \to \mathbb{R}$ is continuous and monotonic over a segment $[a, b] \subset \mathbb{R}$, it then takes all the values within $[\inf(f(a), f(b)), \sup(f(a), f(b))]$.

- **The Rolle theorem**: if f is a function defined over $[a, b] \subset \mathbb{R}$, continuous and differentiable, and if f(a) = f(b), then $\exists c \in]a, b[, f'(c) = 0$.

- **Cauchy's mean value theorem**: If f, g are two functions defined over $[a, b] \subset \mathbb{R}$, continuous over $[a, b]$ and differentiable over $]a, b[$, then $\exists c \in]a, b[$, such that:

$$\big(f(b) - f(a)\big)g'(c) = \big(g(b) - g(a)\big)f'(c)$$

L’Hôpital rule

G. de L’Hôpital
(1661-1704)

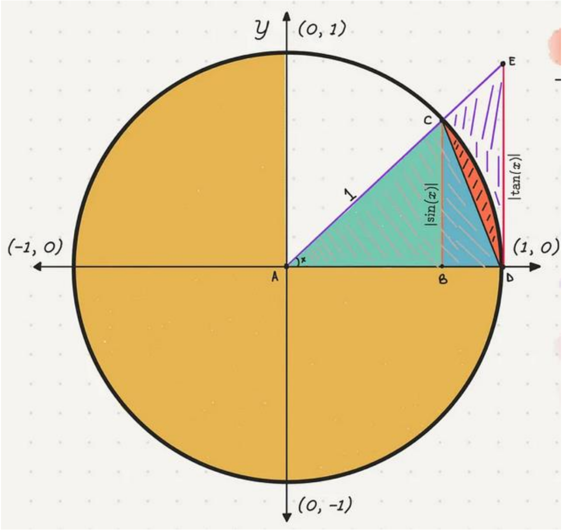
- The Hôpital rule: It states that the limit, when we divide one function by another is the same after we take the derivative of each function (under certain conditions..).

- If :
  - f and g are two functions, differentiable over an interval I, not necessarily at c;
  - g’ is not zero around c (for all $x \neq c$)
  - We have : $\lim_{x \to c} f(x) = \lim_{x \to c} g(x) = 0 \; or \; \pm\infty$
  - $\lim_{x \to c} \frac{f\prime(x)}{g\prime(x)}$ exists:

$$\lim_{x \to c} \frac{f(x)}{g(x)} = \lim_{x \to c} \frac{f'(x)}{g'(x)}$$

- The rule also applies for $x \to \infty$

- Examples:
  - $\lim_{x \to 0} \frac{\sin(x)}{x}$
  - $(\sin(x))'$ from the definition of the differential



Differentiability

- We saw that the differential is a form of linear approximation of a function (linearization): the equality is exact when we take the limit:

$f(x+h) \approx f(x) + hf'(x)$, which we can also write: $f(x+h) = f(x) + hf'(x) + o(h)$

with $\lim_{h \to 0} \frac{o(h)}{h} = 0$

- From the fundamental definition, several operations on the differentiation of functions can be demonstrated:

General rules	Function $y = f(x)$	Derivative $y' = f'(x)$
1. Constant factor	$y = cf(x)$	$y' = cf'(x)$
2. Sum (algebraic) rule	$y = u(x) + v(x)$	$y' = u'(x) + v'(x)$
3. Product rule	$y = u(x)v(x)$	$y' = u'(x)v(x) + u(x)v'(x)$
4. Quotient rule	$y = \frac{u(x)}{v(x)}$	$y' = \frac{u'(x)v(x) - u(x)v'(x)}{v(x)^2}$
5. Chain rule	$y = f[g(x)]$	$y' = \frac{\mathrm{d}f}{\mathrm{d}g} g'(x) = f'(g(x)) \times g'(x)$
6. Inverse functions	$y = f^{-1}(x)$ i.e. $x = f(y)$	$y' = \frac{1}{\mathrm{d}x/\mathrm{d}y} = \frac{1}{f'(y)}$

Or: $(f^{-1})' = \frac{1}{f'(f^{-1}(x))}$

Differentiability

3. Product rule $y = u(x)v(x)$ $y' = u'(x)v(x) + u(x)v'(x)$

$$u(x+h)v(x+h) = \big(u(x) + hu'(x) + o(h)\big)\big(v(x) + hv'(x) + p(h)\big)$$

$$= u(x)v(x) + hu(x)v'(x) + u(x)p(h)$$

$$+ hu'(x)v(x) + h^2u'(x)v'(x) + hu'(x)p(h)$$

$$+ o(h)\big(v(x) + hv'(x) + p(h)\big)$$

$$\Rightarrow \frac{u(x+h)v(x+h) - u(x)v(x)}{h} = u(x)v'(x) + u'(x)v(x)$$

$$\left.\begin{array}{l} + u(x)\dfrac{p(h)}{h} + hu'(x)v'(x) + p(h) \\ + \dfrac{o(h)}{h}\big(v(x) + hv'(x) + p(h)\big) \end{array}\right\} \xrightarrow[h\to 0]{} 0$$

$$\Rightarrow \lim_{h\to 0} \frac{u(x+h)v(x+h) - u(x)v(x)}{h} = u(x)v'(x) + u'(x)v(x)$$

Common functions

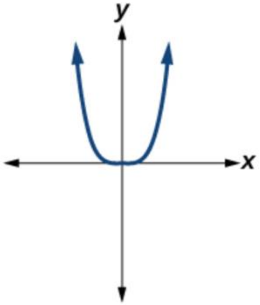
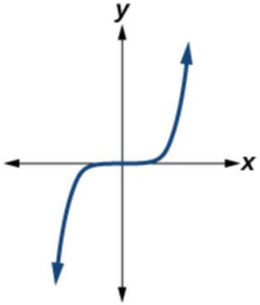
- A *power function* is a function that can be represented in the form $f(x) = kx^{\alpha}$, where k and α are real numbers, and k is known as the *coefficient*.

They are continuous functions and can be differentiated until the derivative is null.

- One can show that from the definition of the differentiability of a function that:

$\forall \alpha \in \mathbb{R}, f'(x) = \alpha k x^{\alpha - 1}$

These functions are the basis of polynomials.

Even power	Odd power
	
$x \to -\infty, f(x) \to \infty$ and $x \to \infty, f(x) \to \infty$	$x \to -\infty, f(x) \to -\infty$ and $x \to \infty, f(x) \to \infty$

- Exponential functions:
  Function of the form $f\colon \mathbb{R}\ (or\ \mathbb{C}) \to \mathbb{R}\ (or\ \mathbb{C})$
  $$f(x) = a^{x}$$

- From the fundamental definition of the differentiability of a function, we can find the derivative of exponential functions, and find a number e for which $(e^{x})' = e^{x}$

- e is defined as: $e = \lim_{n\to\infty}\left(1 + \frac{1}{n}\right)^{n}$

- We can deduct immediately that, defining the function $x \in \mathbb{R}, \ln(x) = (e^{x})^{-1}$, $(\ln(x))' = \frac{1}{x}$.

Common derivatives

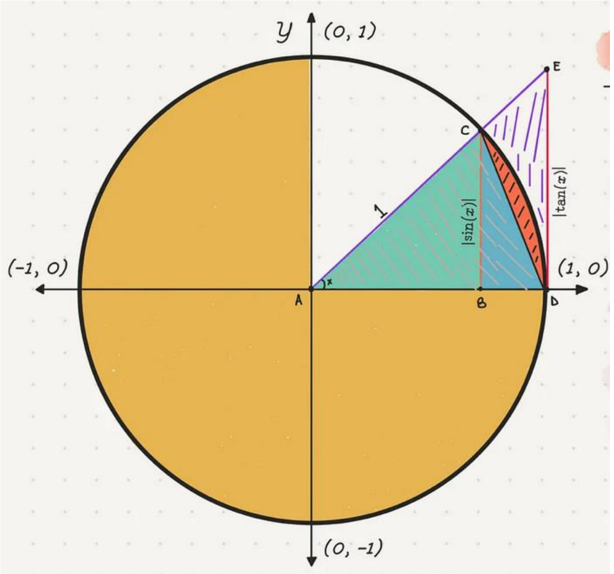
Derivatives of fundamental functions	Function $y = f(x)$	Derivative $y' = f'(x)$
1. Constant factor	$y = \text{constant}$	$y' = 0$
2. Power function	$y = x^n$	$y' = nx^{n-1}$
3. Trigonometric functions	$y = \sin x$	$y' = \cos x$
	$y = \cos x$	$y' = -\sin x$
	$y = \tan x$	$y' = \frac{1}{\cos^2 x} = 1 + \tan^2 x$
	$y = \cot x$	$y' = \frac{-1}{\sin^2 x} = -1 - \cot^2 x$
4. Inverse trigonometric functions	$y = \sin^{-1} x$	$y' = \frac{1}{\sqrt{1-x^2}}$
	$y = \cos^{-1} x$	$y' = -\frac{1}{\sqrt{1-x^2}}$
	$y = \tan^{-1} x$	$y' = \frac{1}{1+x^2}$
	$y = \cot^{-1} x$	$y' = -\frac{1}{1+x^2}$

Common derivatives

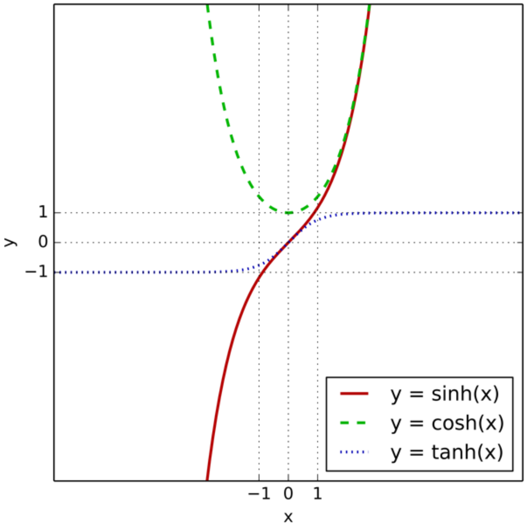
Derivatives of fundamental functions	Function $y = f(x)$	Derivative $y' = f'(x)$
5. Exponential function	$y = e^x$	$y' = e^x$
Logarithmic function	$y = \ln x$	$y' = \frac{1}{x}$
6. Hyperbolic trigonometric functions	$y = \sinh x$	$y' = \cosh x$
	$y = \cosh x$	$y' = \sinh x$
	$y = \tanh x$	$y' = \frac{1}{\cosh^2 x} = 1 - \tanh^2 x$
	$y = \coth x$	$y' = \frac{1}{\sinh^2 x} = 1 - \coth^2 x$
7. Inverse hyperbolic trigonometric functions	$y = \sinh^{-1} x$	$y' = \frac{1}{\sqrt{1+x^2}}$
	$y = \cosh^{-1} x$	$y' = \frac{1}{\sqrt{x^2-1}} \quad (x > 1)$
	$y = \tanh^{-1} x$	$y' = \frac{1}{1-x^2} \quad (\lvert x\rvert < 1)$
	$y = \coth^{-1} x$	$y' = -\frac{1}{x^2-1} \quad (\lvert x\rvert > 1)$

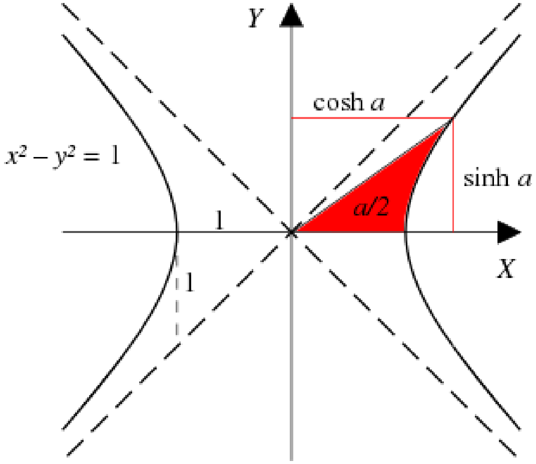
Common derivatives

- Examples: $sin(x),\ a^x, log_a(x), cosh^{-1}(x)$
  - $\frac{d}{dx}(\sin(x)) = cos(x)$
  - $\frac{d}{dx}(a^x) = a^x(\ln(a))$
  - $\frac{d}{dx}\left(log_a(x)\right) = log_a(e)\frac{1}{x}$



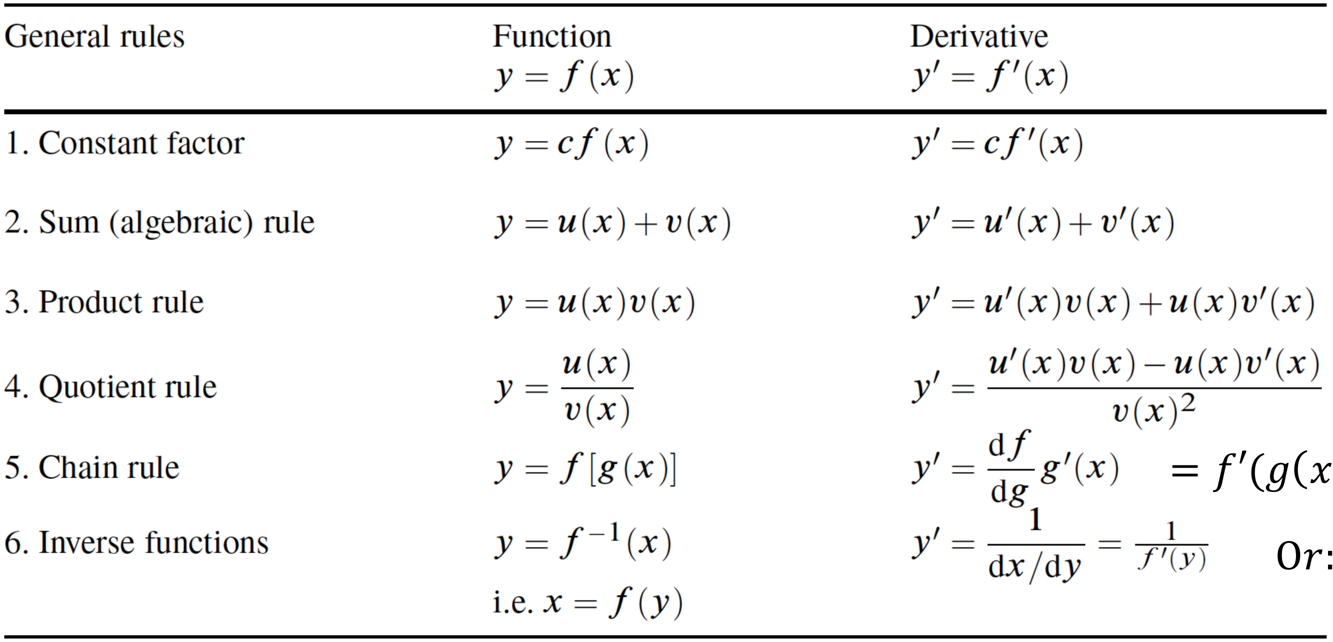
- Hyperbolic functions:
  - $cosh(x) = \frac{e^x + e^{-x}}{2}$
  - $\sinh(x) = \frac{e^x - e^{-x}}{2}$
  - $tanh(x) = \frac{\sinh(x)}{\cosh(x)}$
  - $cosh^2(x) - sinh^2(x) = 1$
  - $\frac{d}{dx}(cosh^{-1}(x)) = \frac{1}{\sqrt{x^2-1}}$





Differentiability

- From the fundamental definition, several operations on the differentiation of functions can be demonstrated



General rules	Function $y = f(x)$	Derivative $y' = f'(x)$
1. Constant factor	$y = cf(x)$	$y' = cf'(x)$
2. Sum (algebraic) rule	$y = u(x) + v(x)$	$y' = u'(x) + v'(x)$
3. Product rule	$y = u(x)v(x)$	$y' = u'(x)v(x) + u(x)v'(x)$
4. Quotient rule	$y = \dfrac{u(x)}{v(x)}$	$y' = \dfrac{u'(x)v(x) - u(x)v'(x)}{v(x)^2}$
5. Chain rule	$y = f[g(x)]$	$y' = \dfrac{\mathrm{d}f}{\mathrm{d}g} g'(x)$
6. Inverse functions	$y = f^{-1}(x)$ i.e. $x = f(y)$	$y' = \dfrac{1}{\mathrm{d}x/\mathrm{d}y} = \dfrac{1}{f'(y)}$

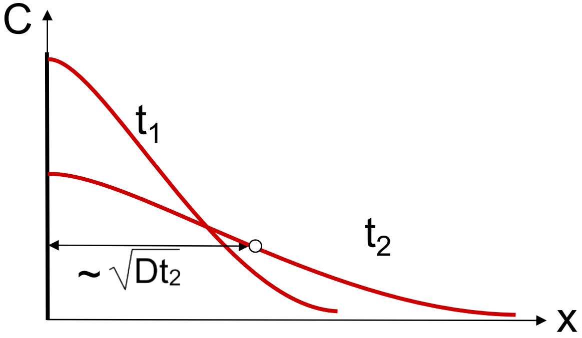
$= f'(g(x)) \times g'(x)$

Or: $(f^{-1})' = \dfrac{1}{f'(f^{-1}(x))}$

- Example: one solution of the diffusion equation: $\frac{\partial c(x,t)}{\partial t} = D \frac{\partial^2 c(x,t)}{\partial x^2}$

Doping Si with P or B to create p-n junctions

$$c(x,t) = \frac{A}{\sqrt{t}} e^{-\frac{x^2}{4Dt}}$$

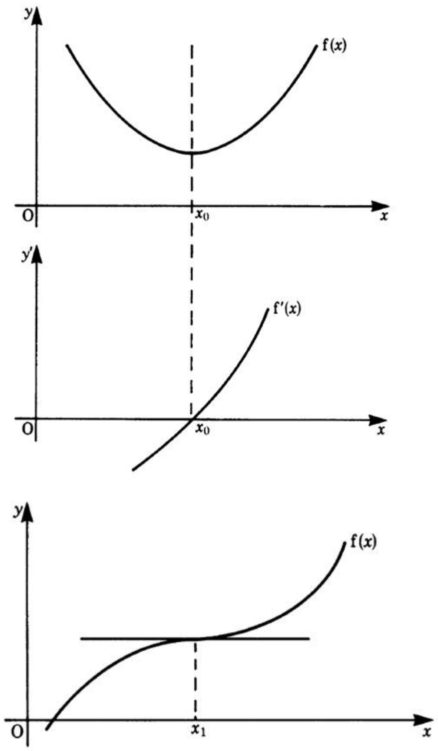


Maximum, minimum, inflexion

- Successive derivatives can help evaluate in a finer way the change of functions, and in particular if they have a maximum or a minimum locally.

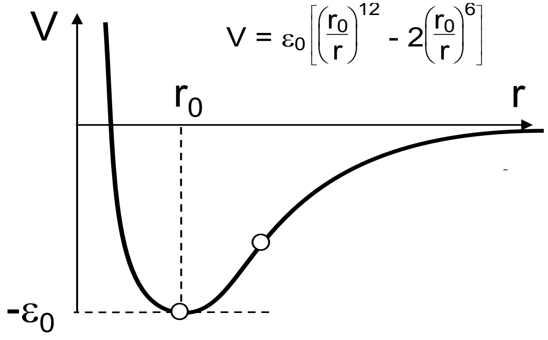
- For a function to have an extremum at a point x_0, it is necessary that $f'(x_0) = 0$. It is however not sufficient.
- It must also be such that $f''(x_0) > 0$ (convex) or $f''(x_0) < 0$ (concave).

- A point of inflexion is such that $f''(x_0) = 0$, marking where the concavity of a function changes.
  We must also have $f'''(x_0) \neq 0$ (for example $f(x) = (x-1)^4$).

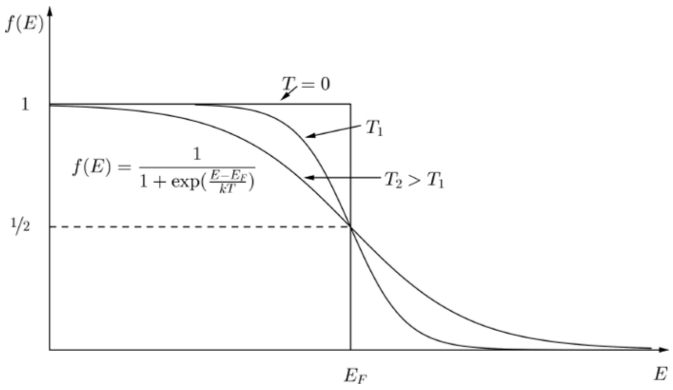


Examples:

Lennard-Jones potential: bonds



Electrons Occupancy

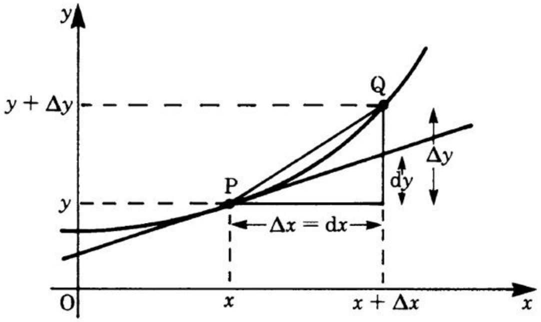


Taylor Series and Taylor expansion

- We saw that the differential is a form of linear approximation of a function (linearization): the equality is exact when we take the limit:

  $f(x+\Delta x) \approx f(x) + f'(x)\Delta x$, which we can also write:

$$f(x+\Delta x) = f(x) + f'(x)\Delta x + \Delta x h(\Delta x) \text{ with } \lim_{\Delta x \to 0} h(\Delta x) = 0$$



- The error is however quickly large as we move away from x. A better approximation can be obtained with a higher degree polynomial

- **Taylor-Lagrange**

  For a function at least n+1 times differentiable ($n \in \mathbb{N}$), defined over an interval $[a, b] \subset \mathbb{R}$,

(The (n+1)th derivative needs to exist only in $]a, b[$), then $\exists c \in \,]a, b[$ such that:

$$f(b) = f(a) + (b-a)f'(a) + \frac{(b-a)^2}{2!}f''(a) + \ldots + \frac{(b-a)^n}{n!}f^{(n)}(a) + \frac{(b-a)^{n+1}}{(n+1)!}f^{(n+1)}(c)$$

- Hint of demo: consider the function

$$\varphi : [a, b] \to \mathbb{R} \quad x \mapsto f(b) - f(x) - (b-x)f'(x) - \cdots - \frac{(b-x)^n}{n!}f^{(n)}(x) - A\frac{(b-x)^{n+1}}{(n+1)!},$$

It is continuous and differentiable.

We have: $\varphi(a) = \varphi(b) = 0$. and $\forall x \in \,]a, b[, \qquad \varphi'(x) = -\frac{(b-x)^n}{n!}f^{(n+1)}(x) + A\frac{(b-x)^n}{n!}$

From Rolle's theorem, $\exists c \in \,]a, b[$ such that $\varphi'(c) = 0$. Hence the result.

Taylor Series and Taylor expansion

- Let’s consider the domain of definition of f, $I \subset \mathbb{R}$, that includes 0, and an arbitrary point x in this interval. We can re-write the Taylor Lagrange polynomial what is called the Maclaurin form (with $c \in]0, x[$):

$$\forall x \in I, f(x) = \sum_{k=0}^{n} \frac{x^k}{k!} f^{(k)}(0) + \frac{x^{n+1}}{(n+1)!} f^{(n+1)}(c)$$

$R_n(x) = \frac{x^{n+1}}{(n+1)!} f^{(n+1)}(c)$ is called the remainder of the Taylor polynomial $\sum_{k=0}^{n} \frac{x^k}{k!} f^{(k)}(0)$.

- This remainder is small, and hence the function is well approximated by the Taylor polynomial, in two situations:

Taylor Expansion

x is close to 0

For all n, the polynomial is a **local** approximation of the function around 0.

The approximation globally improves as the degree of the polynomial increases for small x.

Taylor Series

$n \text{ } is \text{ } large \text{ } (n \to \infty)$

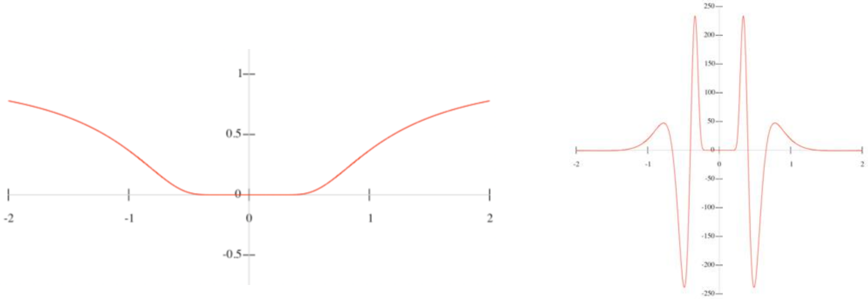
For all x, the polynomial is a **global** approximation of the function over a certain domain where the series $\sum_{k=0}^{\infty} \frac{x^k}{k!} f^{(k)}(0)$

Converges.

Taylor Series

- Taylor series is a wonderful tool to express all functions as polynomials which are regular and easy functions to manipulate.
- For all x, the polynomial is a **global** approximation of the function over a certain domain where the series $\sum_{k=0}^{\infty} \frac{x^k}{k!} f^{(k)}(0)$ converges.

- However, not all functions can be expanded as a Taylor (or Maclaurin) series, and the convergence only happens within certain values of x.



- Examples:
  - $e^{-\frac{1}{x^2}}$ has all its nth differential null at 0.

- One intuitive way to evaluate the convergence is to look at the behavior of the remainder.

- If : $\exists M \in \mathbb{R}, \forall n \in \mathbb{N}, \forall x \in I, \left| f^{(n+1)}(x) \right| \leq M$, then $\forall n \in \mathbb{N}, |R_n(x)| \leq M \frac{x^{n+1}}{(n+1)!} \to 0 \text{ as } n \to \infty$

With two consequences:

- $f(x) = \sum_{k=0}^{n} \frac{x^k}{k!} f^{(k)}(0) + \mathrm{o}(x^n)$ for x small, close to 0.
- The series converges towards f(x): $\left| f(x) - \sum_{k=0}^{n} \frac{x^k}{k!} f^{(k)}(0) \right| \leq M \frac{x^{n+1}}{(n+1)!} \to 0 \text{ as } n \to \infty$
- Hence functions with points of divergence within a domain will be problematic:

$$f(x) = (x-1)^{3/2}$$

Taylor Series - Convergence

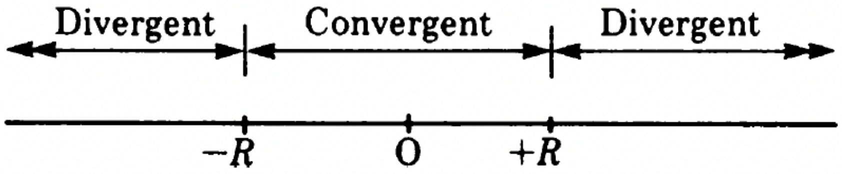
- There are different tests that can assess the convergence of a series:
  - Ratio test: one looks at the behaviour of the ratio of two following sequence number in the series as n goes to infinity.
  - At a point x for a Taylor series, this gives:

$$a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots + a_n x^n + a_{n+1} x^{n+1} + \cdots$$

The ratio is: $\dfrac{a_{n+1} x^{n+1}}{a_n x^n}$

- Taking the limit: $\displaystyle \lim_{n\to\infty} \left| \frac{a_{n+1}}{a_n} x \right| = \frac{|x|}{R}$ where $\displaystyle R = \lim_{n\to\infty} \left| \frac{a_n}{a_{n+1}} \right|$

- The series is absolutely convergent if |x| < R and divergent if |x| > R. Hence a power series is convergent in a definite interval (−R,R) and divergent outside this interval.



- Examples: $e^x, \frac{1}{1-x}$

- Other convergence tests exist like the Cauchy-Hadamar: $\displaystyle \frac{1}{R} = \lim_{n\to\infty} \sqrt[n]{|a_n|}$

Taylor series and expansion

Maclaurin series valid over $\mathbb{R}$

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + ... + (-1)^n \frac{x^{2n}}{(2n)!} + ...$$

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - ... + (-1)^n \frac{x^{2n+1}}{(2n+1)!} + ...$$

$$\arctan(x) = x - \frac{x^3}{3} + \frac{x^5}{5} - ... + (-1)^n \frac{x^{2n+1}}{2n+1} + ...$$

$$\arcsin(x) = x + \frac{1}{2}\frac{x^3}{3} + \frac{1.3}{2.4}\frac{x^5}{5} + ... + \frac{1.3...(2n-1)}{2.4...(2n)}\frac{x^{2n+1}}{2n+1} + ...$$

$$\exp(x) = 1 + \frac{x}{1!} + \frac{x^2}{2!} + ... + \frac{x^n}{n!} + ...$$

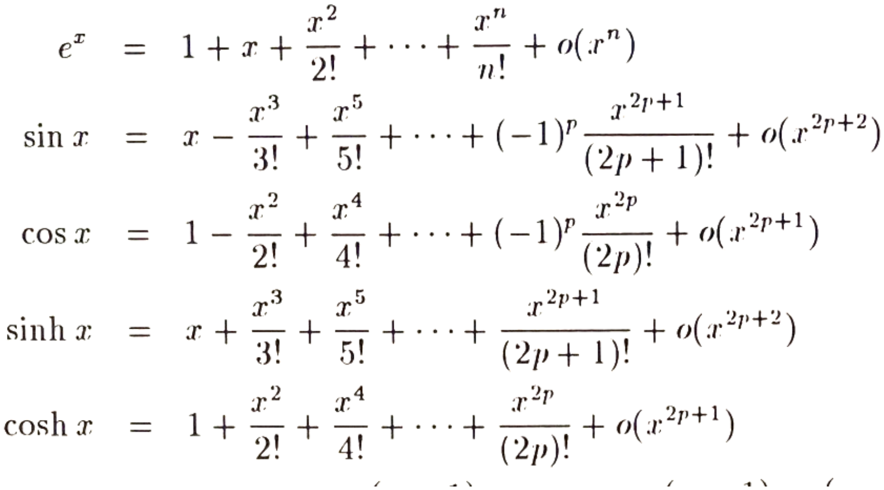
$$\cosh(x) = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + ... + \frac{x^{2n}}{(2n)!} + ...$$

$$\sinh(x) = x + \frac{x^3}{3!} + \frac{x^5}{5!} + ... + \frac{x^{2n+1}}{(2n+1)!} + ...$$

$$(1+x)^\alpha = 1 + \frac{\alpha}{1!}x + \frac{\alpha(\alpha-1)}{2!}x^2 + ... + \frac{\alpha(\alpha-1)...(\alpha-n+1)}{n!}x^n + ...$$

$$\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - ... + (-1)^{n-1}\frac{x^n}{n} + ...$$

Taylor expansion **around 0 at the order n**:



$$\begin{aligned}
e^x &= 1 + x + \frac{x^2}{2!} + \cdots + \frac{x^n}{n!} + o(x^n) \\
\sin x &= x - \frac{x^3}{3!} + \frac{x^5}{5!} + \cdots + (-1)^p \frac{x^{2p+1}}{(2p+1)!} + o(x^{2p+2}) \\
\cos x &= 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \cdots + (-1)^p \frac{x^{2p}}{(2p)!} + o(x^{2p+1}) \\
\sinh x &= x + \frac{x^3}{3!} + \frac{x^5}{5!} + \cdots + \frac{x^{2p+1}}{(2p+1)!} + o(x^{2p+2}) \\
\cosh x &= 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \cdots + \frac{x^{2p}}{(2p)!} + o(x^{2p+1})
\end{aligned}$$

Euler formula:

- These expressions are true also for complex arguments !
- Comparing: $e^{ix}, \cos(x)\,, i\sin(x)$, one sees quickly that indeed: $e^{ix} = \cos(x) + i\sin(x)$

Taylor Expansion

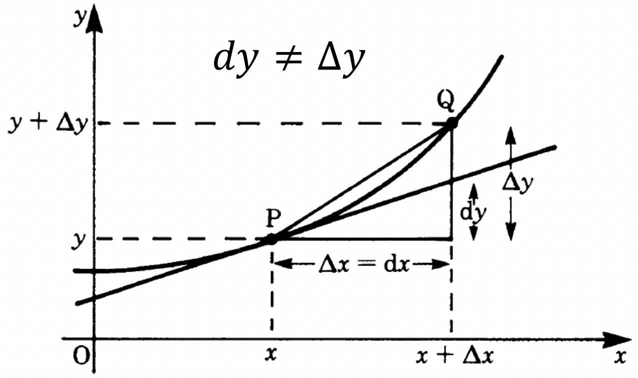
- Taylor expansion does not worry about convergence: as long as a function is n-times differentiable around an argument, it can be approximated (more or less well) by the Taylor expansion.

- Note that it is an approximation ! The differential is an exact value of a slope when, one takes the limit.

$f(x+\Delta x) \approx f(x) + f'(x)\Delta x$, which we can also write:

$$f(x+\Delta x) = f(x) + f'(x)\Delta x + \Delta x h(\Delta x) \text{ with } \lim_{\Delta x \to 0} h(\Delta x) = 0$$

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} \qquad \Delta y = f(x+\Delta x) - f(x)$$



- From the Taylor series, one can extract the expansion to a first few orders:

Example for the second order: $f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + o(h^2)$

- The approximation improves usually at higher order:

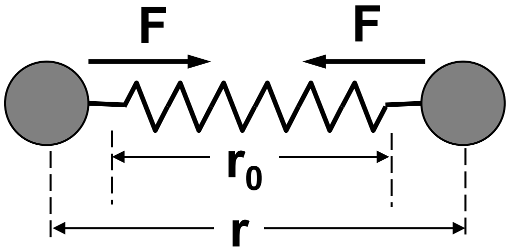
    - Zero-th order: the function is constant, locally approximated to its value at 0 (or other)
    - First order: linear approximation that is very often used in engineering;
    - Second order: quadratic approximation also widely used, often when f'(0) = 0.

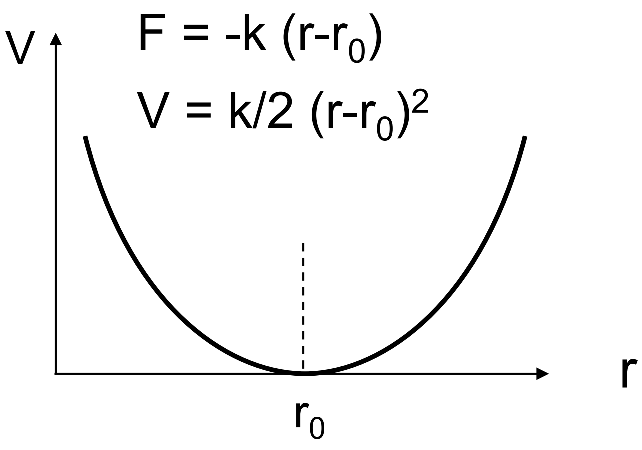
Physical representation of chemical bonds

A simple model to physically apprehend the bond between atoms: the Lennard-Jones potential.

A Conservative force (the work done on an object does not depend on the object’s path) can be derived from this potential:

$$\vec{F} = -\overrightarrow{grad}\, V$$



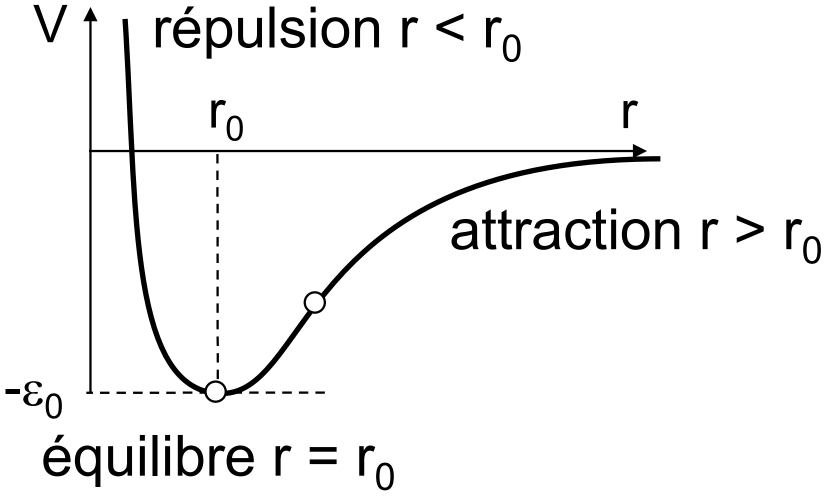


$F = -k\,(r-r_0)$

$V = k/2\,(r-r_0)^2$

Potential of Lennard-Jones:

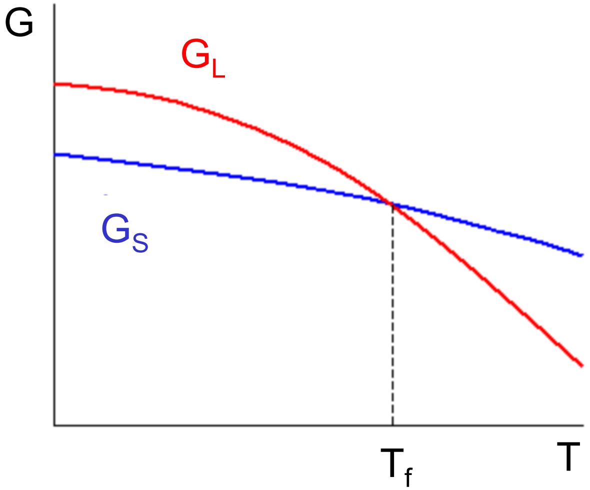
$$V = \varepsilon_0\left[\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^{6}\right]$$

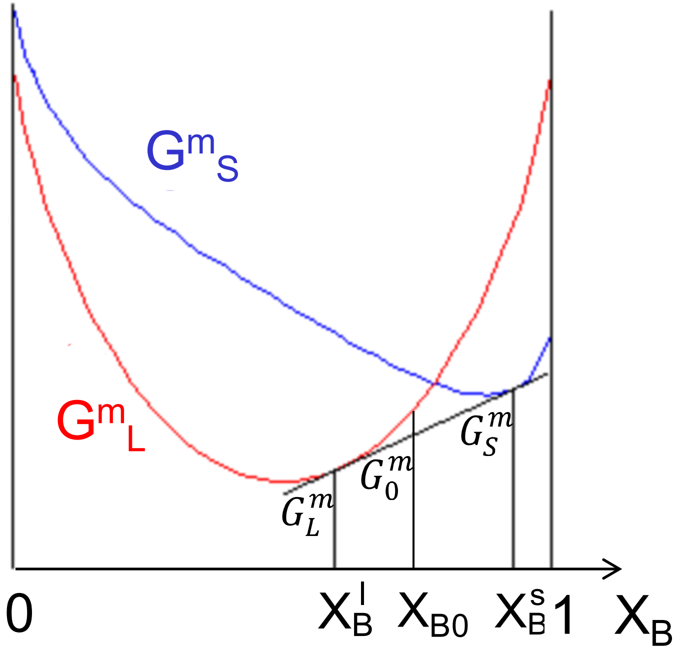


Tangents in Materials Science: Binary Systems

- The equilibrium of a thermodynamic system is driven by the minimization of the Gibbs free energy (at T and P constant).

- For a unitary system, the molar free enthalpy as a function of temperature looks like this:



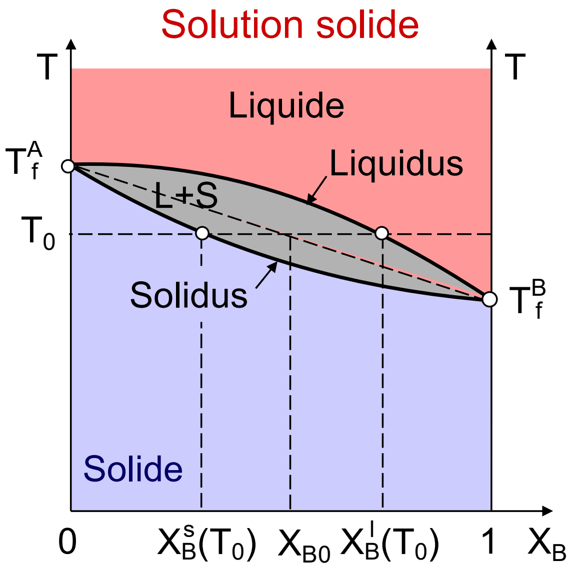


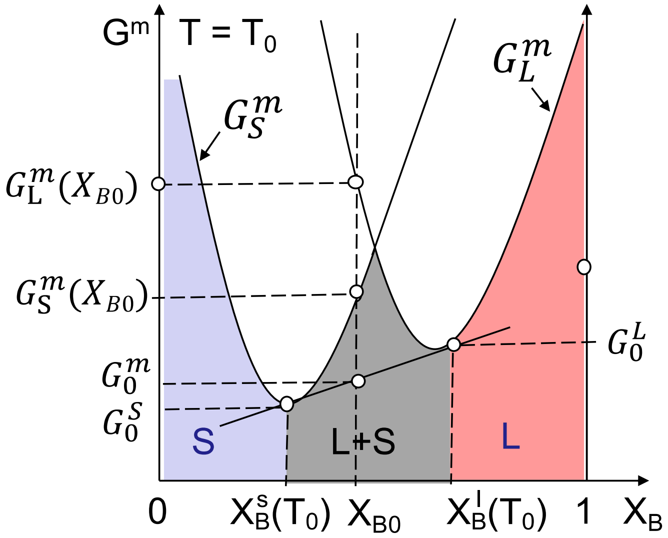
- For a binary system of species A and B (Cu and Ni for example) with $n_{tot} = n_A + n_B$

$$X_{A0} = \frac{n_A}{n_{tot}} \qquad X_{B0} = \frac{n_B}{n_{tot}}$$

- the system can separate into two different phases of different composition to minimise the free enthalpy.

Binary Systems with full Solubility





- At T = T_0, the Gibbs free energy of the liquid solution at X_{B0} is higher than the one for the solid phase. We can then expect the system to be in the solid state.
- The system has however an alternative possibility to further reduce its free energy: put a fraction χ_S in the solid phase, and a fraction χ_L in the liquid phase (with $\chi_S + \chi_L = 1$).
- By taking the common tangent of the molar Gibbs energy for the solid (G_S^m) and the liquid (G_L^m), we can find the proportion of B in the liquid ($X_B^L(T_0)$) and the solid ($X_B^S(T_0)$) phases.
- The molar Gibbs free energy is then given by:

L

$$G_0^m = \chi_S G_0^S + \chi_L G_0^L < G_S^m(X_{B0})$$

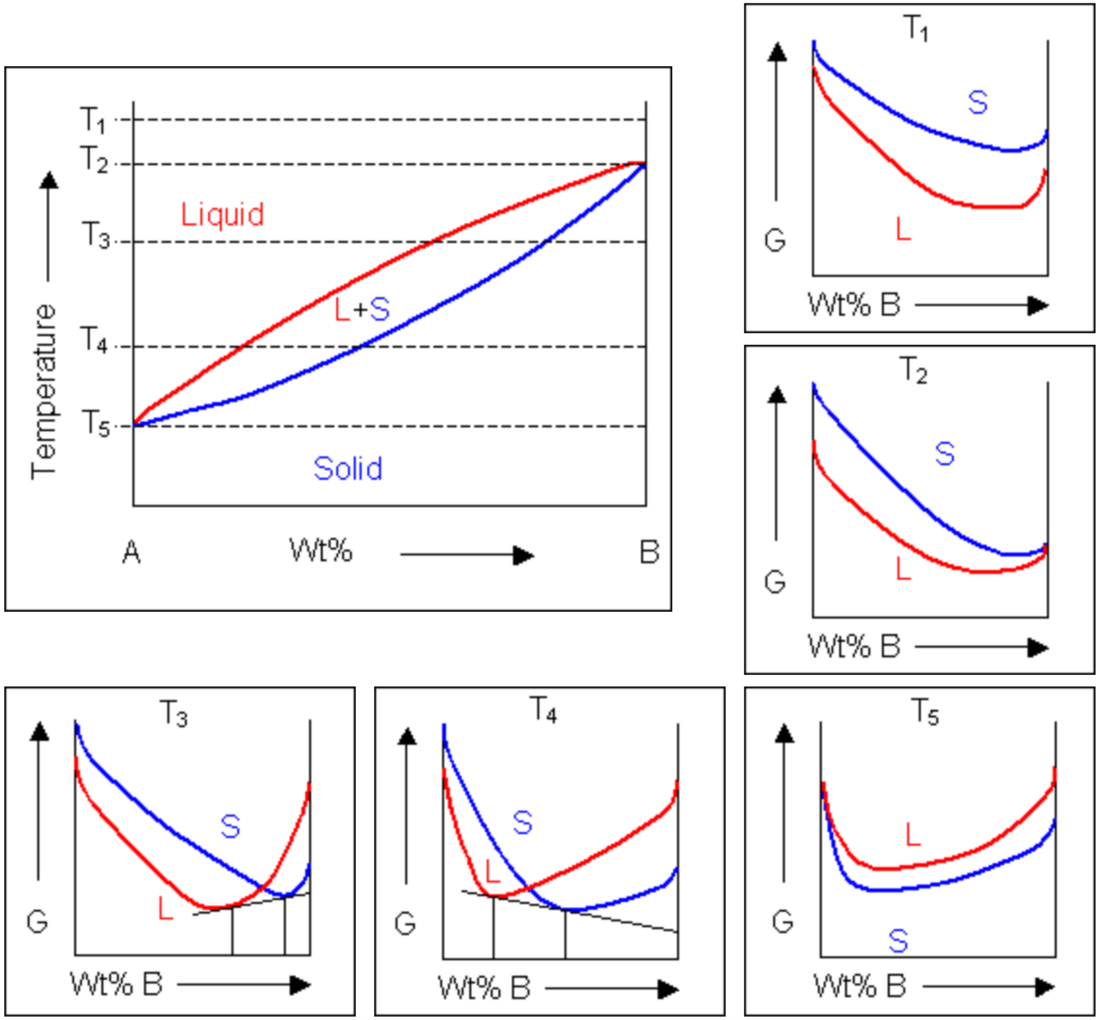
- By computing the slope of the tangent, we have:

$$G_0^m = \frac{X_B^L - X_{B0}}{X_B^L - X_B^S} G_0^S + \frac{X_{B0} - X_B^S}{X_B^L - X_B^S} G_0^L$$

- Which enables to recover the lever rule.

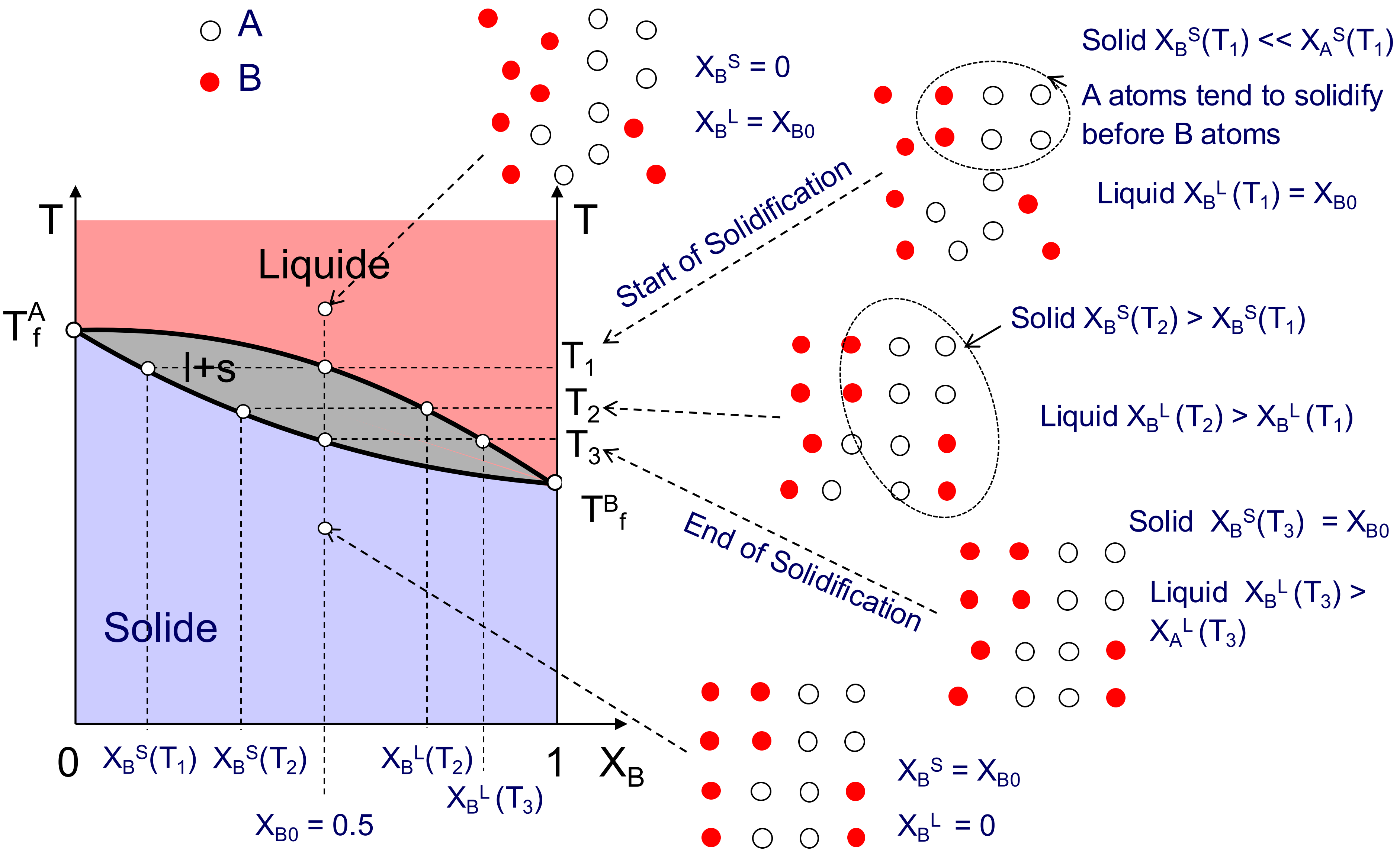
Binary Systems with full Solubility

- From the Gibbs free energy curves as a function of X_B at different temperatures, we can then reconstruct the phase diagram for all temperatures.



https://www.doitpoms.ac.uk/tlplib/phase-diagrams/printall.php

Binary Systems with full Solubility



$X_B{}^S = 0$

$X_B{}^L = X_{B0}$

Start of Solidification

Solid $X_B{}^S(T_1) << X_A{}^S(T_1)$

A atoms tend to solidify before B atoms

Liquid $X_B{}^L(T_1) = X_{B0}$

Solid $X_B{}^S(T_2) > X_B{}^S(T_1)$

Liquid $X_B{}^L(T_2) > X_B{}^L(T_1)$

End of Solidification

Solid $X_B{}^S(T_3) = X_{B0}$

Liquid $X_B{}^L(T_3) > X_A{}^L(T_3)$

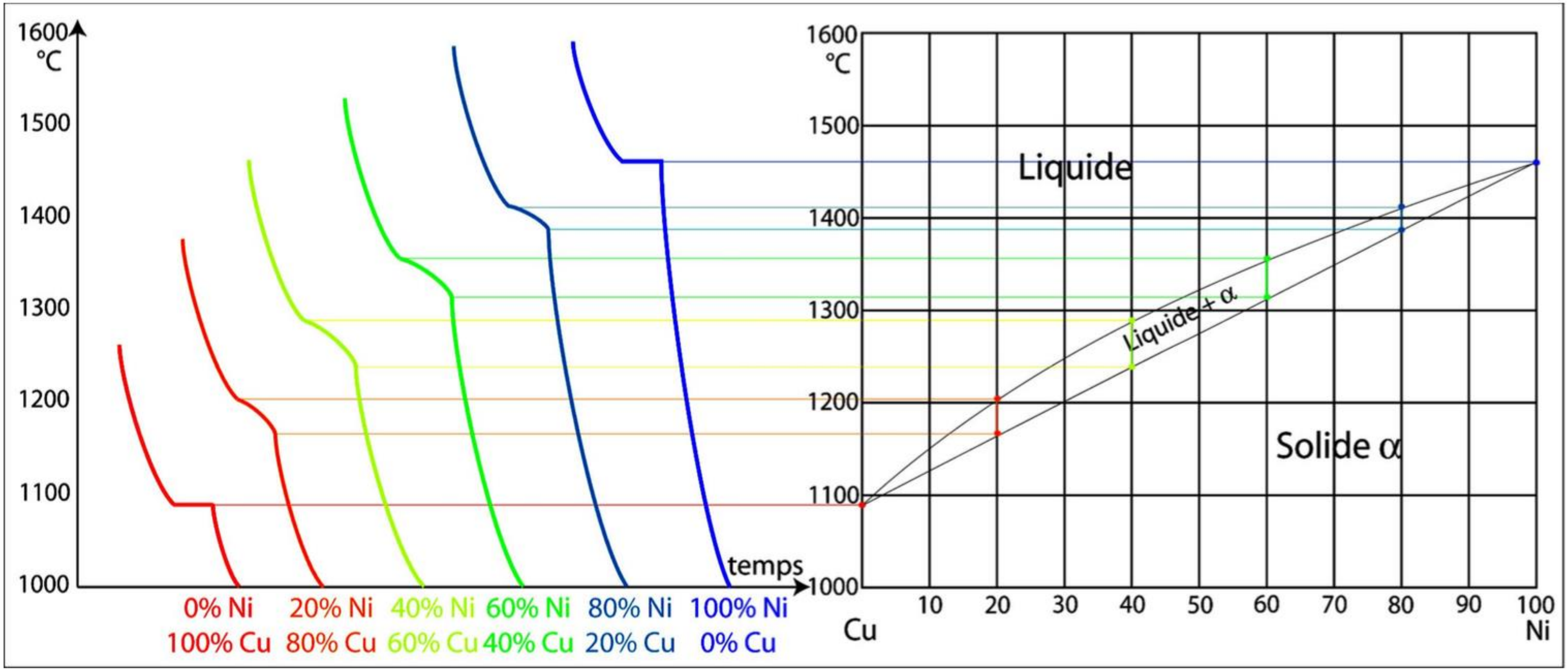
$X_B{}^S = X_{B0}$

$X_B{}^L = 0$

Binary Systems with full Solubility

Example: solidification curves for the diagram Cu-Ni that enables to create the phase diagram.

Note that contrary to unitary systems, the phase change do not occur at a single T.



SUMMARY

- We presented the concept of functions and defined limits, continuity and derivability.
- We focused on differentiability and in particular the tangent of a function.
- We showed how the fundamental definition of the differentiability of a function can be used to find the derivative of some common functions.
- We reminded the L'Hôpital rule.
- We introduced Taylor expansion and Taylor series.
- We introduced the need for the common tangent construction in phase diagrams, and gave an example of an exponential function in the Lennard-Jones potential.
- <u>Next week</u>
  - We will discuss parametric functions and integration.
  - We will also discuss multi-variable functions
  - We will derive the diffusion equation