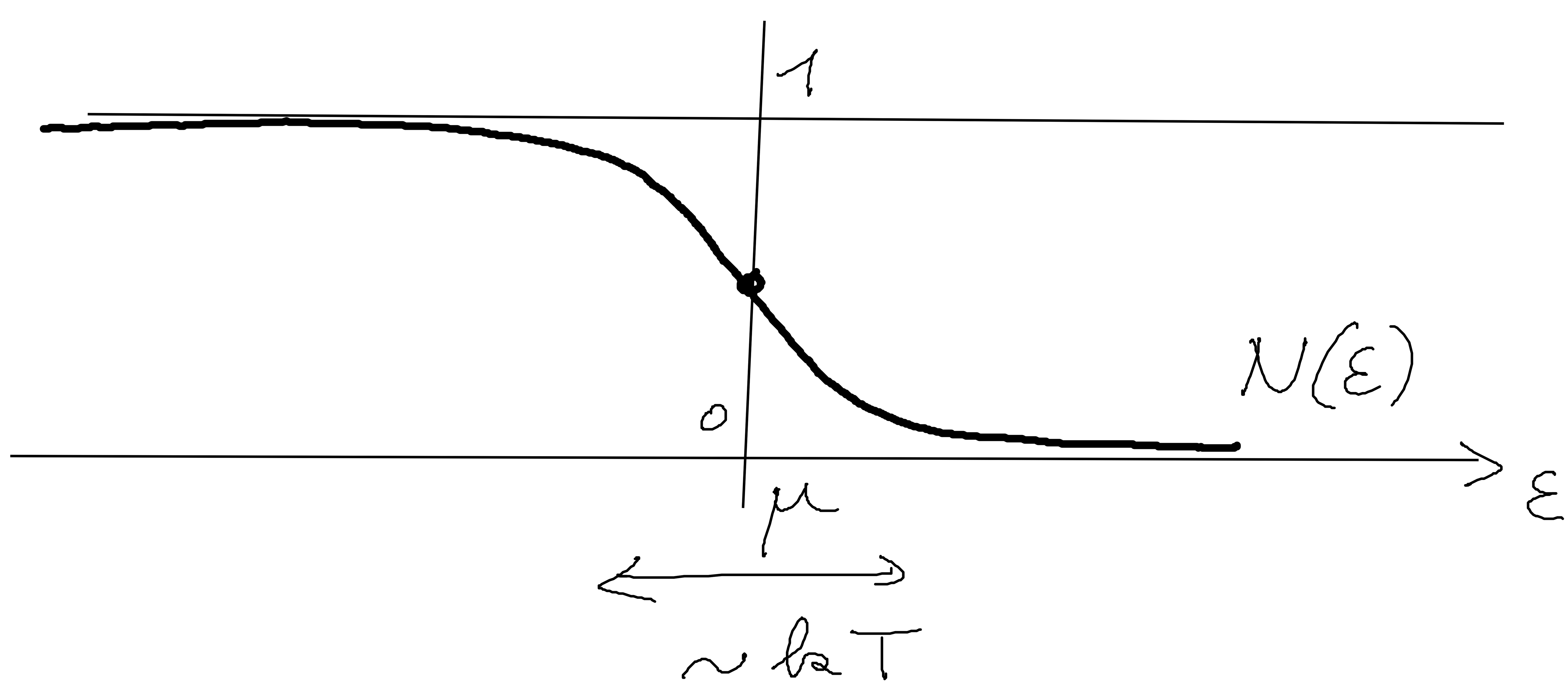
Expansion de Sommerfeld

μ : potentiel chimique

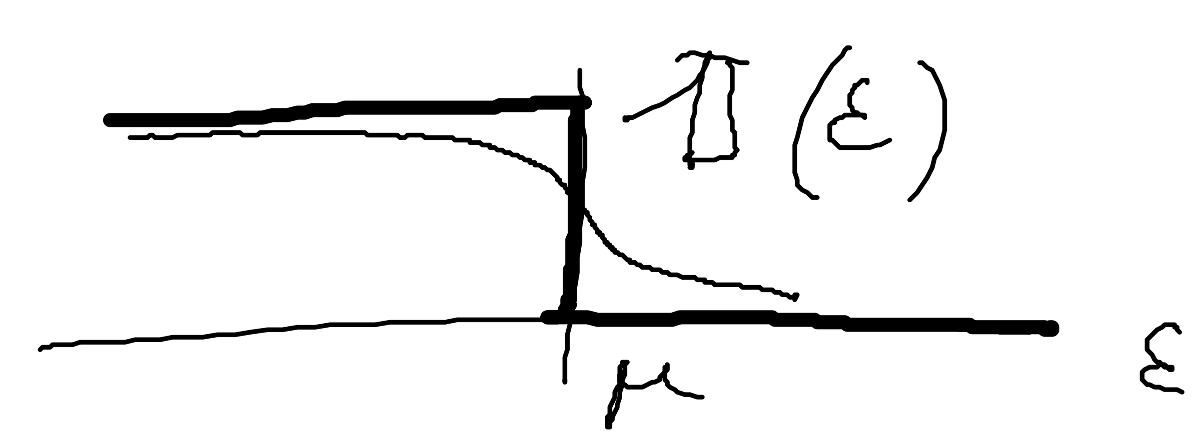
$\beta = \frac{1}{k_B T}$,

$$N(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$: distribution de Fermi

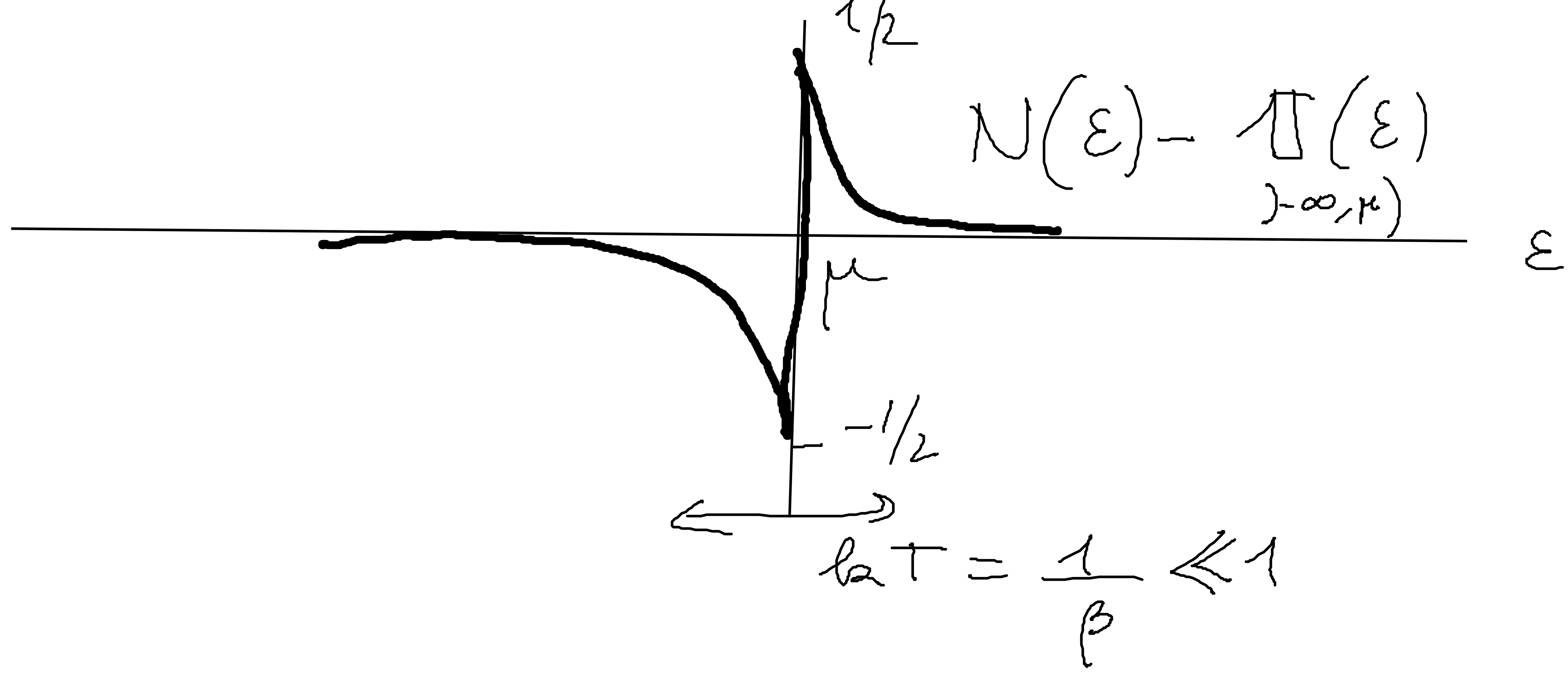


Pour $\beta \to \infty \iff T \to 0$,

$$N(\varepsilon) = \mathbb{1}_{]-\infty,\mu[}(\varepsilon).$$



(appelée fonction indicatrice)



. Posons le changement de variables

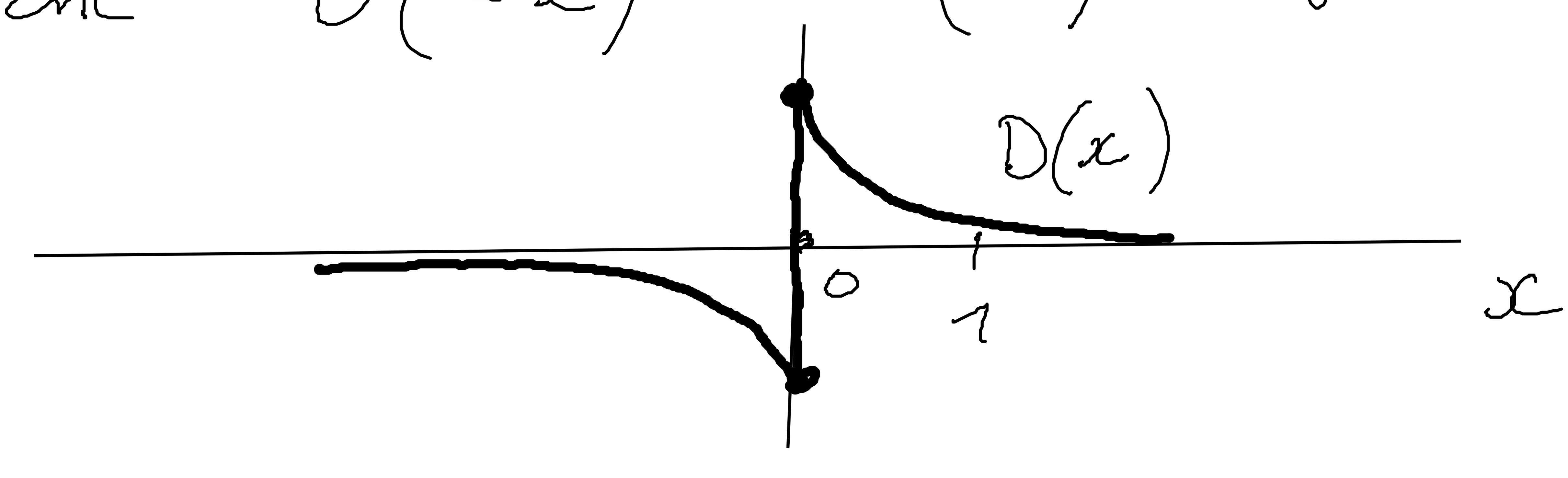
$$\varepsilon \longrightarrow x = \beta(\varepsilon - \mu) \iff \varepsilon = \frac{x}{\beta} + \mu$$

et $D(x) = N(\varepsilon) - \mathbb{1}(\varepsilon)$

si $x < 0$, $D(x) = \dfrac{1}{e^{x}+1} - 1 = \dfrac{-e^{x}}{e^{x}+1} = \dfrac{-1}{1+e^{-x}}$

si $x > 0$, $D(x) = \dfrac{1}{1+e^{x}}$

Donc $D(-x) = -D(x)$: fonction impaire



• Soit $u(\varepsilon)$ une fonction "test"

$$\int_{\mathbb{R}} u(\varepsilon) N(\varepsilon)\, d\varepsilon = \int_{\mathbb{R}} u(\varepsilon) \mathbb{1}_{]-\infty,\mu[}(\varepsilon)\, d\varepsilon + \int_{\mathbb{R}} u(\varepsilon) D(x)\, d\varepsilon$$

$$= \int_{-\infty}^{\mu} u(\varepsilon)\, d\varepsilon + \int_{\mathbb{R}} u\left(\frac{x}{\beta}+\mu\right) D(x) \frac{dx}{\beta}$$

Considérons le 2ème terme.

Pour $\beta \gg 1, \Leftrightarrow \frac{1}{\beta} \ll 1,$

$$u\left(\mu+\frac{x}{\beta}\right) = u(\mu) + u'(\mu)\frac{x}{\beta} + O\left(\frac{1}{\beta^2}\right)$$

alors

$$\int_{\mathbb{R}} u\left(\frac{x}{\beta}+\mu\right) D(x) \frac{dx}{\beta} = \frac{u(\mu)}{\beta} \underbrace{\int D(x)\, dx}_{=0 \text{ car } D \text{ impaire}}$$

$$+ \frac{u'(\mu)}{\beta^2} \int x D(x)\, dx + O\left(\frac{1}{\beta^3}\right)$$

or $\displaystyle\int_0^{\infty} \frac{x}{1+e^x}\, dx = \frac{\pi^2}{12}$ donc $\displaystyle\int_{\mathbb{R}} x D(x)\, dx = \frac{\pi^2}{6}$

donc

$$\boxed{\int_{\mathbb{R}} u(\varepsilon) N(\varepsilon)\, d\varepsilon = \int_{-\infty}^{\mu} u(\varepsilon)\, d\varepsilon + \frac{u'(\mu)}{\beta^2}\frac{\pi^2}{6} + O\left(\frac{1}{\beta^3}\right)}$$