Lecture 4

Chain rule: $f(g(x))$

$h(x) = (x^2+1)^2 + 1$

$f(x) = x^2+1$

$g(x) = x^2+1$

$h(x) = f(g(x)) = f(f(x))$

$$\frac{d\, f(g(x))}{dx} = \frac{dg}{dx} \cdot \frac{df}{dx}(g(x)) = f'(g)\, g'$$

$$Z = \cancel{\sum_{i=1}^{N}} e^{-a\varepsilon_i}$$

$$f(a) = e^{a}$$

$$g(a) = -a\varepsilon_i$$

$$\frac{d}{da} e^{-a\varepsilon_i} = \underbrace{e^{-a\varepsilon_i}}_{f'(g)} \cdot \underbrace{-\varepsilon_i}_{g'}$$

$$\frac{dZ}{da} = \frac{d}{da} \sum_{i=1}^{N} e^{-a\varepsilon_i} = \sum_{i=1}^{N} \frac{d}{da} e^{-a\varepsilon_i}$$

$$= -\sum_{i=1}^{N} \varepsilon_i e^{-a\varepsilon_i}$$

$$\frac{d}{dx}\frac{1}{f(x)} = \frac{d}{dx} g(f(x))$$

$$g(x) = \frac{1}{x} = x^{-1}$$

$$\frac{dg}{dx} = -\frac{1}{x^2}$$

$$-\frac{f'(x)}{(f(x))^2}$$

$$\frac{d}{dx}\frac{1}{1+e^{ax}}$$

$$= \frac{-ae^{ax}}{(1+e^{ax})^2}$$

Back to differentials

$$\frac{df}{dx} = m \iff df = m\,dx$$

$$\underset{\text{response}}{df} = \underbrace{\left(\frac{df}{dx}\right)}_{\text{sensitivity}} dx$$

$$\int d(fg) = \int g\, df + \int f\, dg$$

$$\|$$

$$fg = \int g\, df + \int f\, dg$$

$$\text{“}\int u\, dv = uv - \int v\, du\text{”}$$

$$\int \frac{df}{dx}\, dx = f$$

→ mutivariable calculus

$$f(x,y) = (x^2+1)y^2$$

take derivatives of f

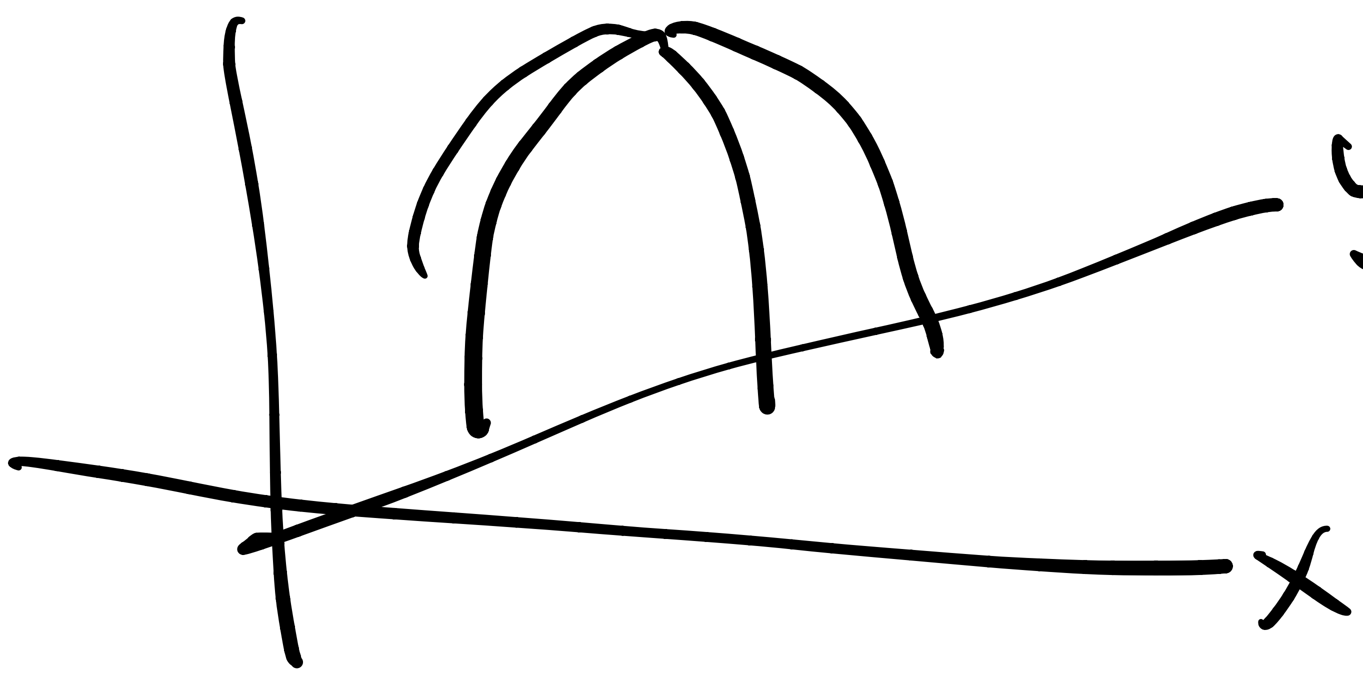
w.r.t. x or y, keeping the other const.

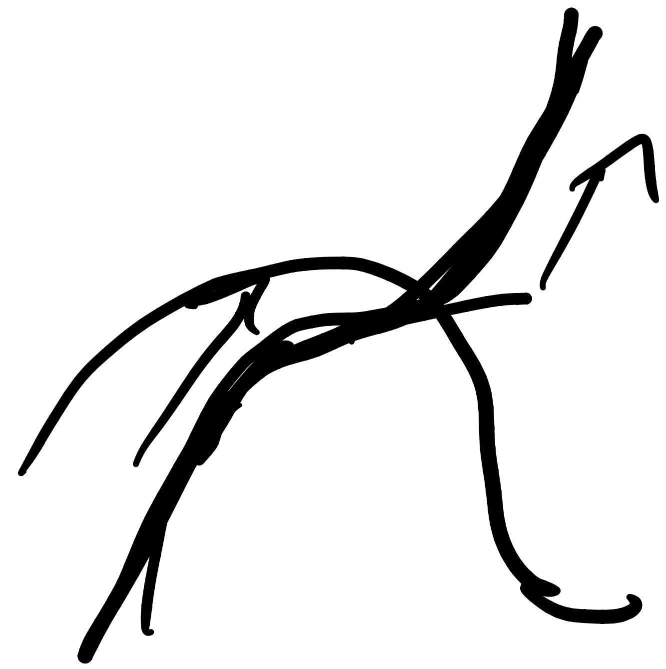
$$\left(\frac{\partial f}{\partial x}\right)_y = y^2 \frac{d}{dx}(x^2+1) = 2x\,y^2$$

$$\left(\frac{\partial f}{\partial y}\right)_x = (x^2+1)\frac{d}{dy}(y^2) = 2y\,(x^2+1)$$

Max or min →

all partial derivatives are 0





for "regular" functions, take partial derivatives in any order

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right)$$

$f(x,y)$, what is df

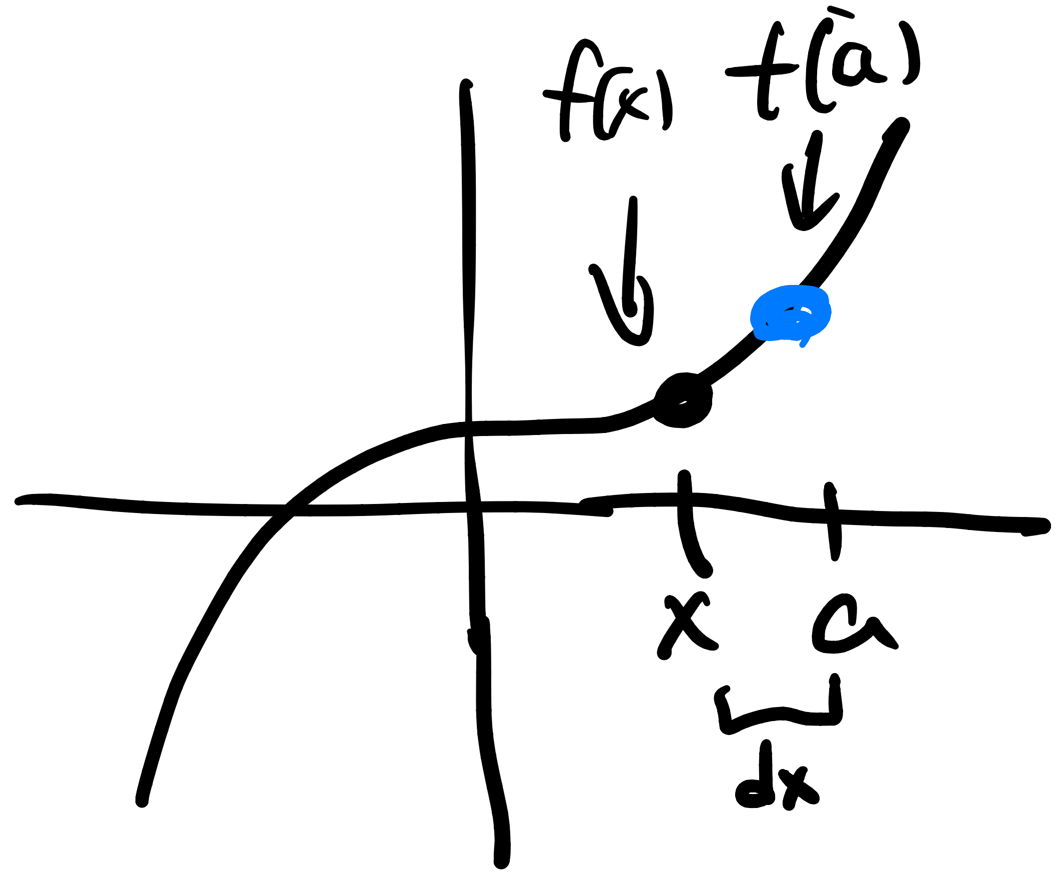
$$df = \left(\frac{\partial f}{\partial x}\right)_y dx + \left(\frac{\partial f}{\partial y}\right)_x dy$$

total differential

$$\frac{df}{dx} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x} = f'(x)$$

$$df = f(x+\Delta x) - f(x) = f'(x)\,\Delta x$$

Taylor series



$a = x + dx$

$$f(x+dx) = f(x) + dx\left(\frac{df}{dx}\right) + \frac{1}{2}(dx)^2\left(\frac{d^2f}{dx^2}\right)$$

$$+ \ldots$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{\partial^n f}{\partial x^n}\right)(dx)^n$$

$$f(x+dx,\ y+dy)$$

$$= f(x,y) + dx\left(\frac{\partial f}{\partial x}\right)_y + dy\left(\frac{\partial f}{\partial y}\right)_x$$

$$+ \frac{1}{2}\underline{dx}^2\left(\frac{\partial^2 f}{\partial x^2}\right)_y + \frac{1}{2}\underline{(dy)}^2\left(\frac{\partial^2 f}{\partial y^2}\right)_x$$

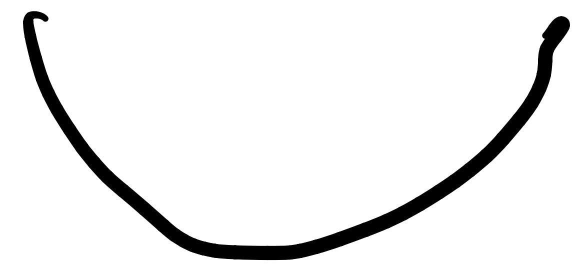
very small

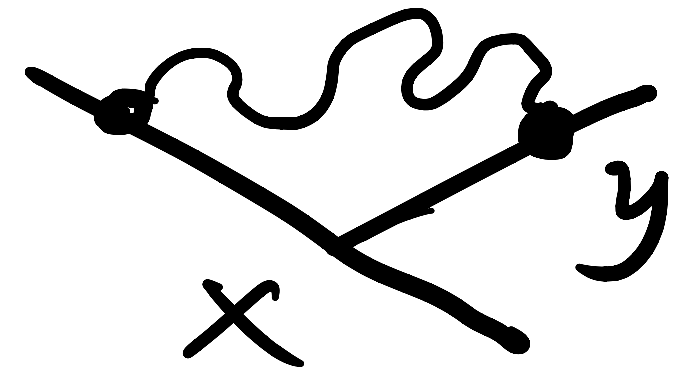
$$+ \underline{dxdy}\left(\frac{\partial^2 f}{\partial x \partial y}\right)$$

$$+ \dots$$

$$df = f(x+dx,\ y+dy) - f(x,y) = dx\left(\frac{\partial f}{\partial x}\right)_y + dy\left(\frac{\partial f}{\partial y}\right)_x$$

$$\int_{\substack{x_1 \to x_2 \\ y_1 \to y_2}} df = \int_{\text{path}} \left(\frac{\partial f}{\partial x}\right)_y dx + \int_{\text{path}} \left(\frac{\partial f}{\partial y}\right) dy$$





$\overset{?}{=}$

$f(x_2, y_2) - f(x_1, y_1)$

If you can write this total derivative formula for "f"

f is a "state function"

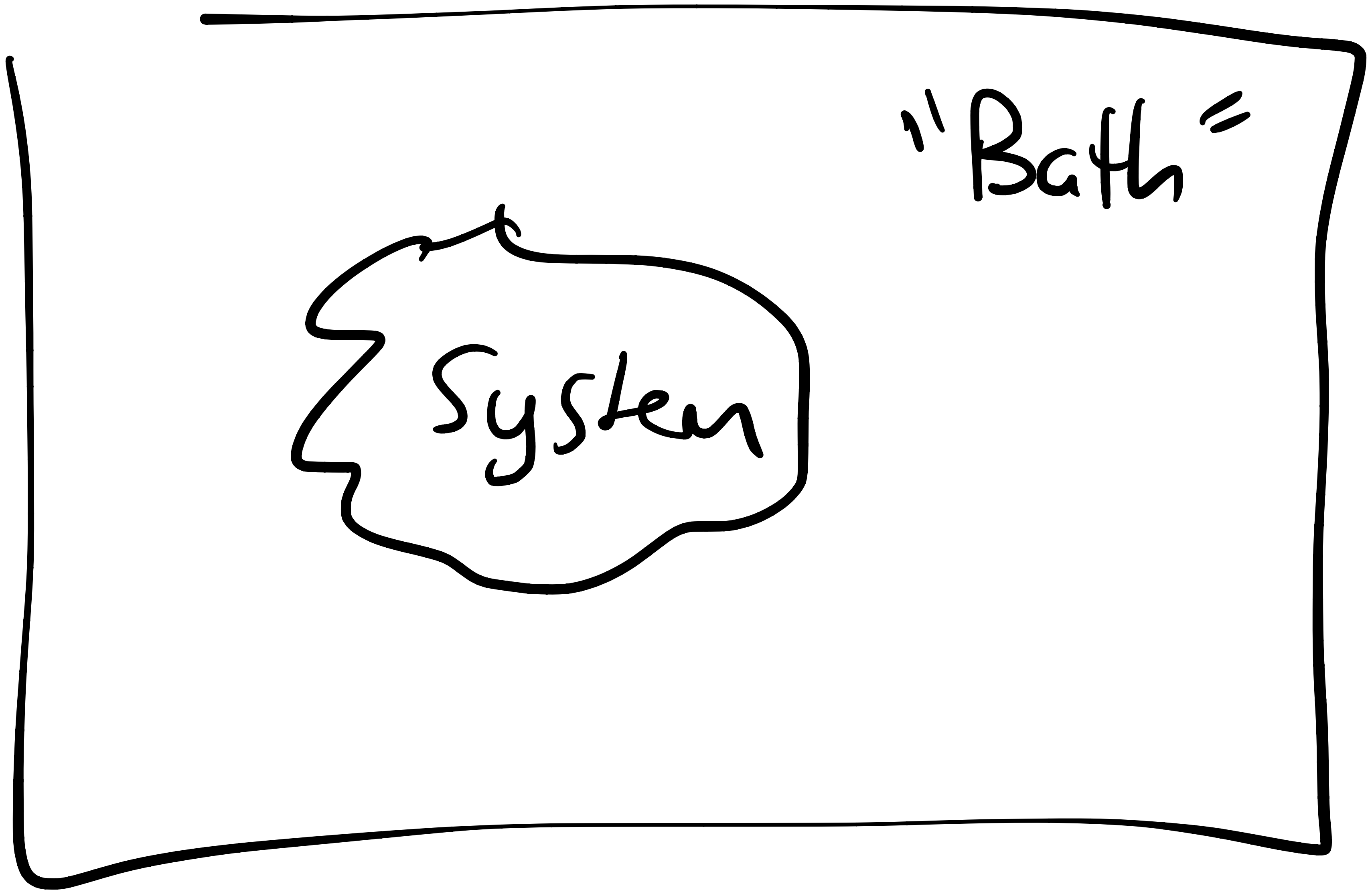
Thermodynamics : introduction

heat → work

Major concepts : equilibrium

↳ state of system isn't changing

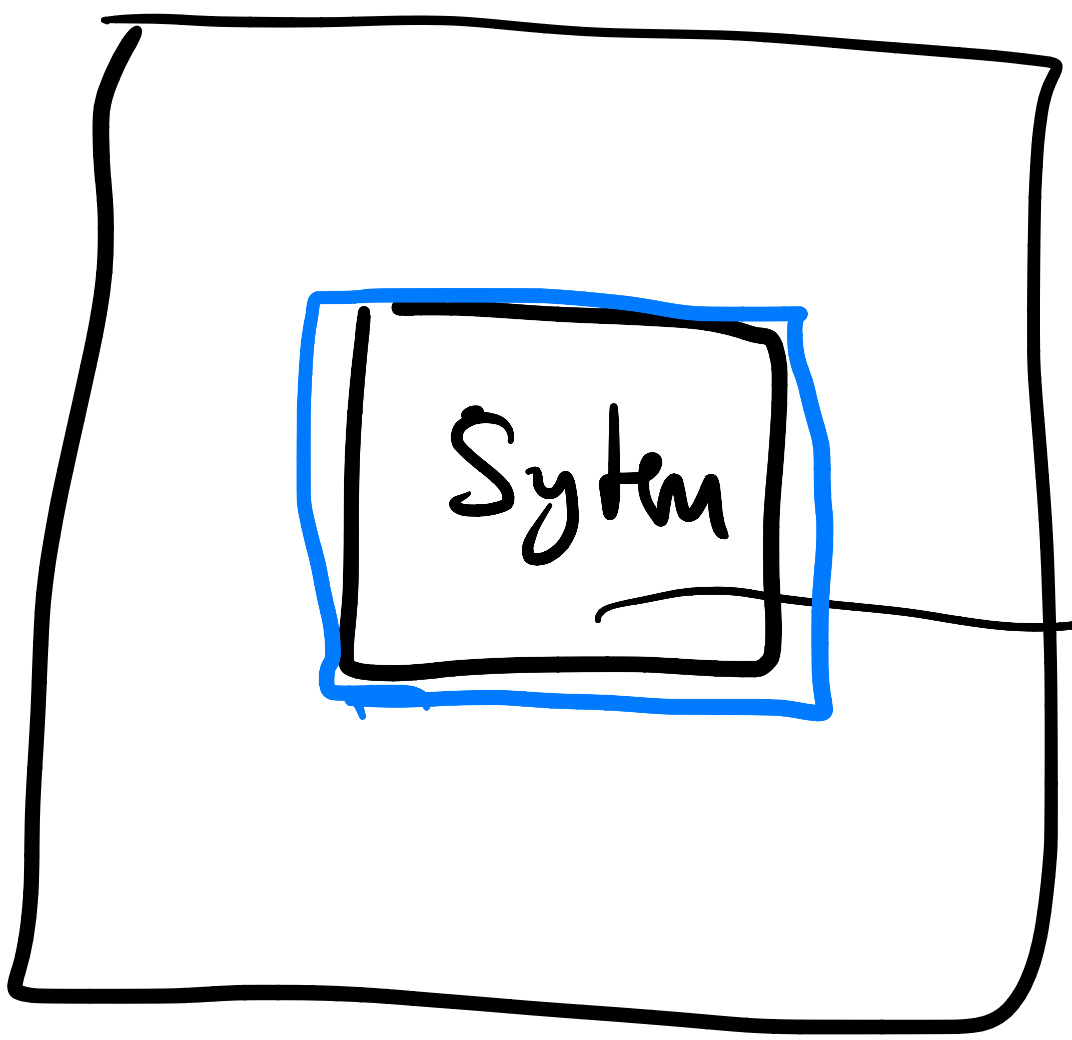
Key : divide the universe into system + surroundings



"Boundary"

System-bath coupling

System big, boundary negligible



V, N mc's

"isolated system"

nothing in or out

Eg $\rightarrow$ Universe is isolated

isolated system w/ N mcs

density $= \frac{N}{V}$ mass density $\frac{mN}{V}$

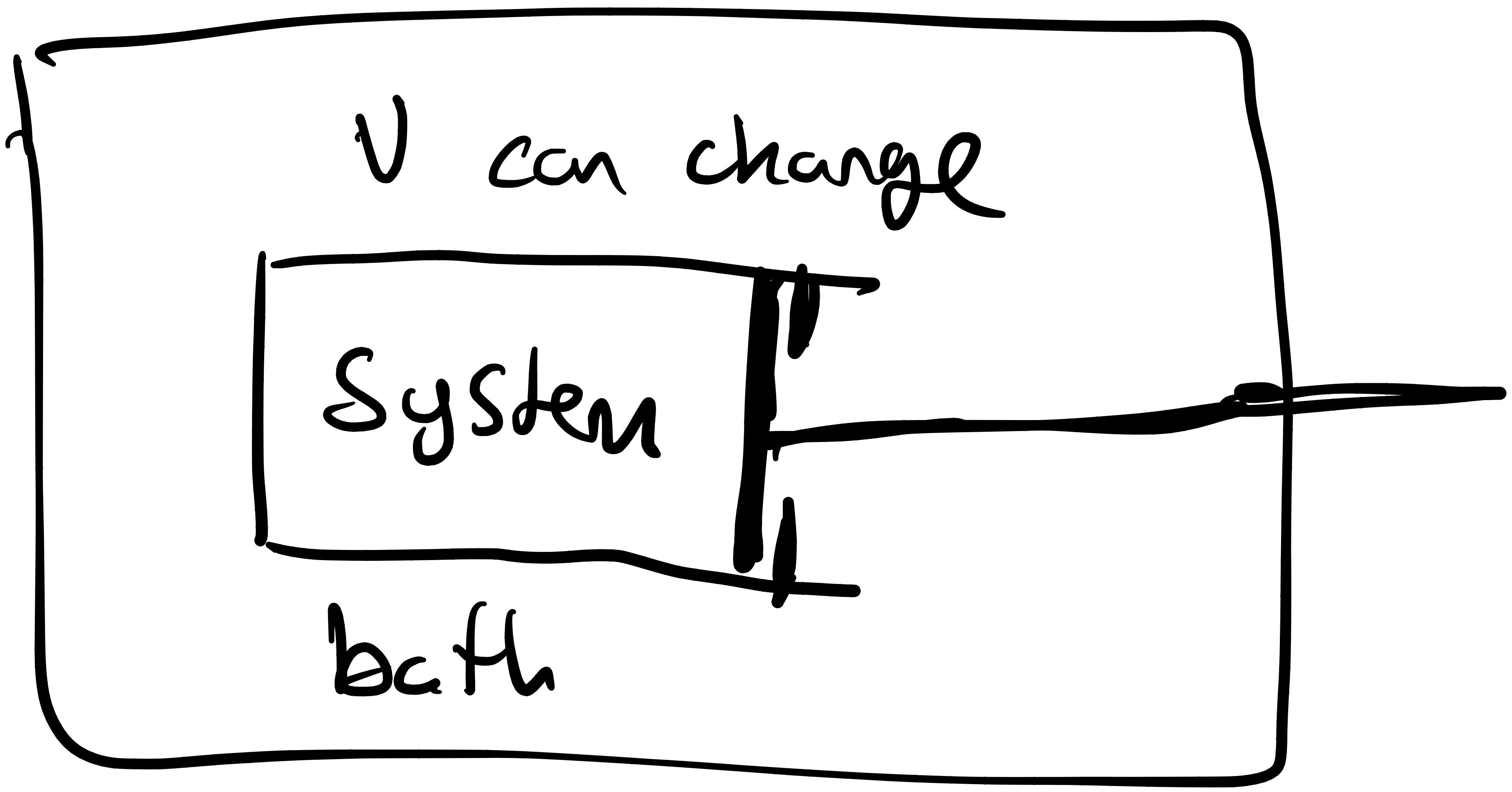
Newton's equations, $F=ma$ $\Big\}$ $\rightarrow$ constant E

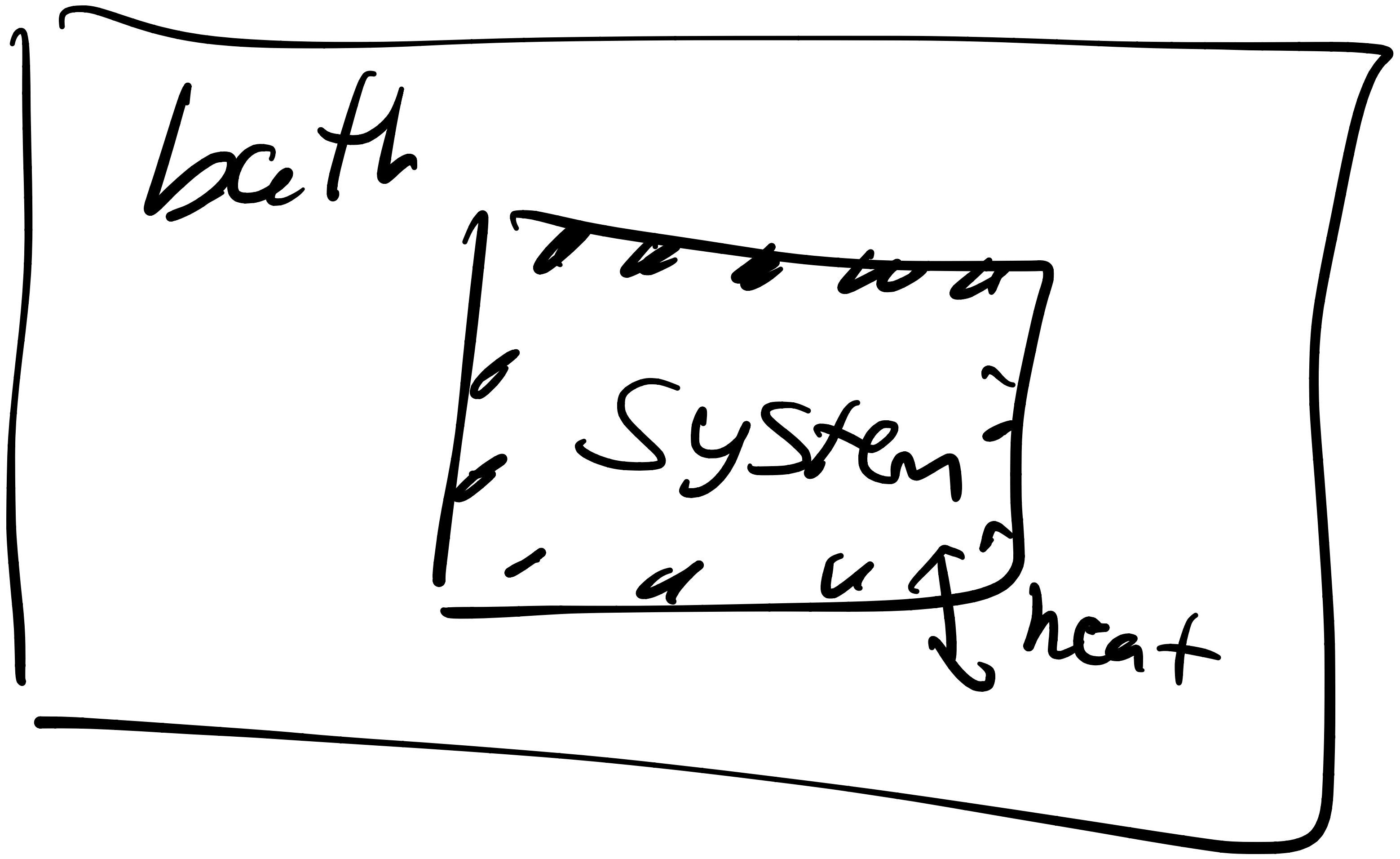
or S.E. $H\Psi = E\Psi$

Isolated: N, V, E are constant

What can we change

We can allow, N, V or E to change





energy can flow

→ turn out

$N, V, \underline{\underline{T}}$