Stationary Points 2

The criterion to find the stationary points of a multi-variable fn $f(x_1, x_2, \cdots, x_N)$ is

$$\boxed{df = 0}$$

① Without any constraint ~

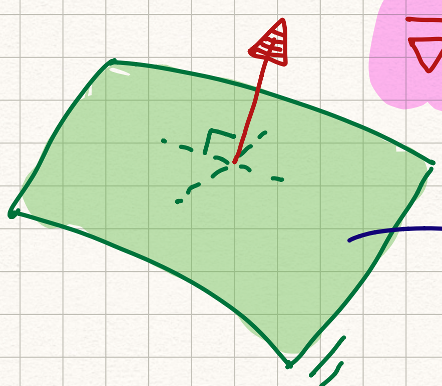
$$df = \vec{\nabla} f \cdot \underbrace{d\vec{r}}_{\text{arbitrary}} \longrightarrow \boxed{\vec{\nabla} f = 0}$$

② With constraint $\phi(x_i) = 0$ ~

From the constraint $\phi(x_i) = 0 \longrightarrow \boxed{d\phi = \vec{\nabla}\phi \cdot d\vec{r} = 0}$

$\boxed{\vec{\nabla} f \parallel \vec{\nabla}\phi}$

$d\vec{r}$ can only move on the surface !



$\phi(x_i) = 0$

Lagrange multiplier

$$df = \vec{\nabla} f \cdot \underbrace{d\vec{r}}_{\text{not arbitrary}} \longrightarrow \boxed{\vec{\nabla} f + \lambda \vec{\nabla}\phi = 0}$$

Shannon Entropy

also known as information entropy

For a coin with the probability distribution

$X = 1 \quad P_1 = p$

$X = 0 \quad P_0 = 1 - p$

$$P_1 + P_0 = 1$$

Conservation of probability

How can one characterize the uncertainty of the random variable X?

$$\sigma = \left\langle \ln \frac{1}{p} \right\rangle = \sum_\alpha P_\alpha \ln \frac{1}{P_\alpha}$$

$$\rightarrow \quad \sigma = -\sum_\alpha P_\alpha \ln P_\alpha$$

Shannon entropy

example a fair coin $P_1 = P_0 = \frac{1}{2}$

$$\sigma = -\frac{1}{2}\ln\frac{1}{2} - \frac{1}{2}\ln\frac{1}{2} = -\ln\frac{1}{2} = \ln 2$$

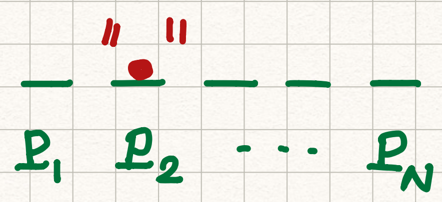
example an biased coin $P_1 = 1,\ P_0 = 0$

$$\sigma = -1 \ln 1 - 0 \ln 0 = 0$$

$$\lim_{x \to 0^+} x \ln x = 0$$

Thermal Equilibrium

When a system reaches thermal equilibrium, its entropy becomes maximum



N states

$$\sigma = -\sum_{\alpha=1}^{N} p_\alpha \ln p_\alpha$$

with the constraint

$$\sum_{\alpha=1}^{N} p_\alpha = 1$$

Making use of Lagrange multiplier,

$$\sigma^* = \sigma + \lambda \left(\sum_{\alpha=1}^{N} p_\alpha - 1 \right)$$

$$\frac{\partial \sigma^*}{\partial p_i} = 0 \longrightarrow -\ln p_i - p_i \cdot \frac{1}{p_i} + \lambda = 0$$

$$\ln p_i = \lambda - 1, \qquad p_i = e^{\lambda - 1} = \text{const.}$$

Substitute back into the constraint $\sum_\alpha p_\alpha = 1$ and the criterion for maximizing entropy is

$$p_i = \frac{1}{N}$$ — microcanonical ensemble

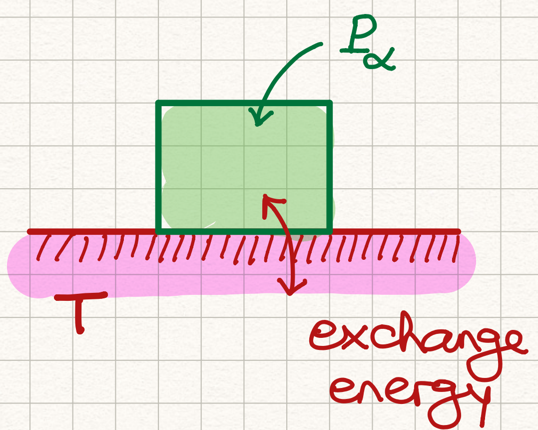
And, the maximum entropy is

$$\sigma_{max} = -\frac{1}{N} \ln \frac{1}{N} \times N = -\ln \frac{1}{N} = \ln N$$

It can be shown that the thermal entropy S is related to σ_{max} (not σ in general)

$$S = k\sigma_{max} = k \ln N$$

For a system with thermal contact to reservoir, the constraints are different ☺



$$\sum_\alpha P_\alpha = 1$$

$$\sum_\alpha P_\alpha E_\alpha = U$$

additional constraint

Again, applying Lagrange multipliers to find the maximum entropy ☺

$$\sigma^* = \sigma + \lambda_1 \left(\sum_\alpha P_\alpha - 1 \right) + \lambda_2 \left(\sum_\alpha P_\alpha E_\alpha - U \right)$$

$$\frac{\partial \sigma^*}{\partial p_i} = 0 \qquad -\ln p_i - p_i \cdot \frac{1}{p_i} + \lambda_1 + \lambda_2 E_i = 0$$

$$\ln p_i = (\lambda_1 - 1) + \lambda_2 E_i \longrightarrow p_i = e^{\lambda_1 - 1} e^{\lambda_2 E_i}$$

Substitute into the constraint $\sum_\alpha p_\alpha = 1$

$$p_i = \frac{e^{\lambda_2 E_i}}{\sum_\alpha e^{\lambda_2 E_\alpha}} = \frac{1}{Z} e^{-E_i/kT}$$

absolute temp

① It turns out $\lambda_2 = -\frac{1}{kT}$!

② $Z = \sum_\alpha e^{-E_\alpha/kT}$ is the partition fn.

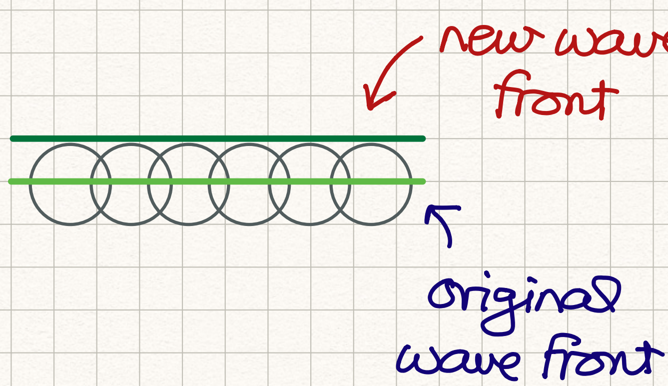
The probability distribution obtained in above is the famous Boltzmann distribution:

$$p(E_i) = \frac{1}{Z} e^{-E_i/kT}$$

The higher-energy states are exponentially rare to find. This is the underlying reason for scientific phenomena @ diff energy scales.

Finding Envelopes

Remember Huygens principle taught in high school? What is the math to find the wave front from those of the wavelets?



= envelope of the wave fronts of the wavelets!

Let us start analyzing a family of curves

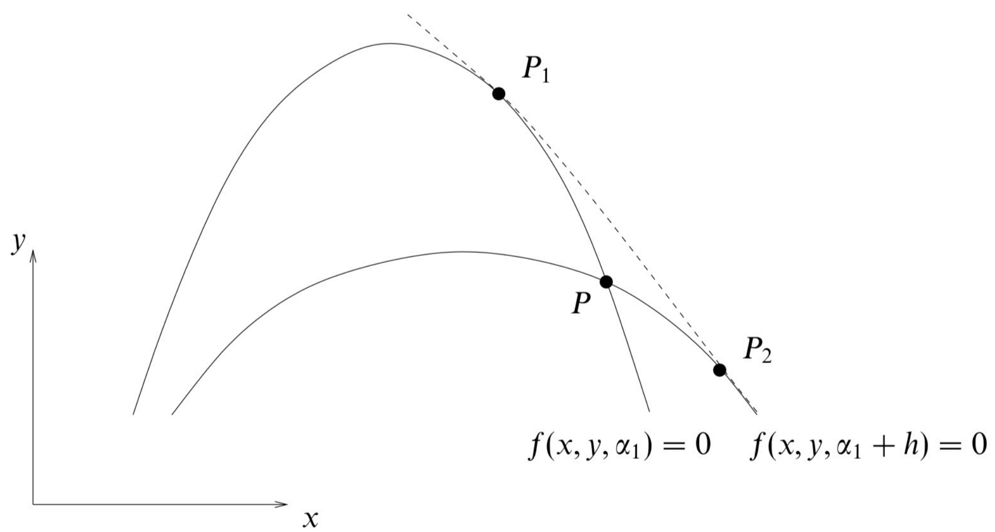


Figure 5.4 Two neighbouring curves in the xy-plane of the family $f(x, y, \alpha) = 0$ intersecting at P. For fixed α_1, the point P_1 is the limiting position of P as $h \to 0$. As α_1 is varied, P_1 delineates the envelope of the family (broken line).

Riley, Hobson, Bence (3rd edition)

The intersecting point P satisfies

$$f(x,y;\alpha)=0 \quad \& \quad f(x,y;\alpha+d\alpha)=0$$

Expanding the 2^{nd} equation ~

$$f(x,y;\alpha+d\alpha) = \overbrace{f(x,y;\alpha)}^{0} + \frac{\partial f}{\partial \alpha}\, d\alpha$$

$$\longrightarrow \quad \frac{\partial f}{\partial \alpha}(x,y;\alpha)=0$$

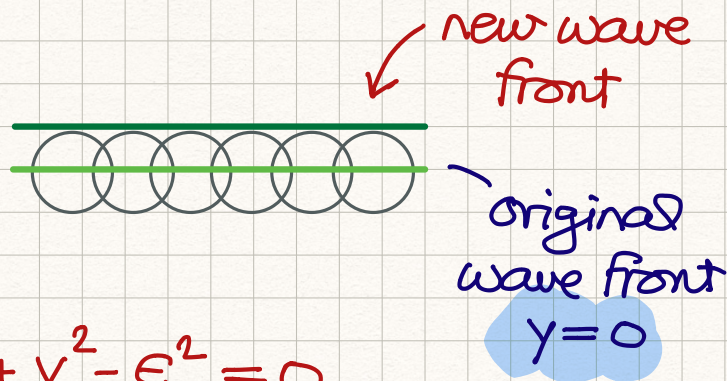
Thus, the envelope can be found by eliminating the parameter α in the equations:

$$f(x,y;\alpha)=0, \quad \frac{\partial f}{\partial \alpha}(x,y;\alpha)=0$$

example Huygens Principle

family of curves:

$$(x-\alpha)^2 + y^2 = \epsilon^2$$



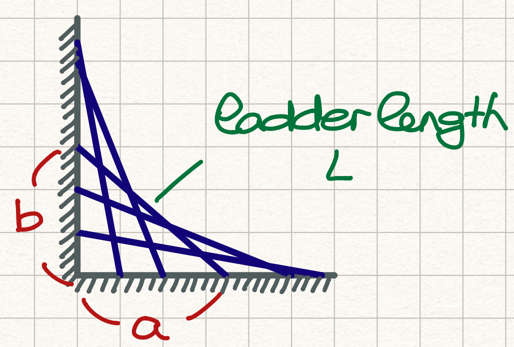
$$\longrightarrow \quad f(x,y;\alpha) = (x-\alpha)^2 + y^2 - \epsilon^2 = 0$$

$$\frac{\partial f}{\partial \alpha} = 0 \quad \longrightarrow \quad -2(x-\alpha)=0$$

It simply gives $x = \alpha$. Substitute it into $f(x, y; \alpha) = 0$ to eliminate the parameter α.

$$\underbrace{\cancel{(\alpha - \alpha)^2}}_{\to 0} + y^2 - \epsilon^2 = 0 \quad \longrightarrow \quad \boxed{y = \pm \epsilon}$$

example Sliding Ladder



The family of curves:

$$\frac{x}{a} + \frac{y}{b} = 1$$

where a, b satisfy

$$a^2 + b^2 = L^2$$

It is convenient to express the parameters as

$$\begin{aligned} a &= L\cos\theta \\ b &= L\sin\theta \end{aligned} \quad \longrightarrow \quad \frac{x}{L\cos\theta} + \frac{y}{L\sin\theta} = 1$$

angular parameter θ

$$f(x, y; \theta) = \frac{x}{L\cos\theta} + \frac{y}{L\sin\theta} - 1 = 0$$

$$\frac{\partial f}{\partial \theta} = 0 \quad \longrightarrow \quad \frac{x}{\cancel{L}} \frac{\sin\theta}{\cos^2\theta} - \frac{y}{\cancel{L}} \frac{\cos\theta}{\sin^2\theta} = 0$$

$$x\frac{\sin\theta}{\cos^2\theta} = y\frac{\cos\theta}{\sin^2\theta} \rightarrow \frac{x}{y} = \frac{\cos^3\theta}{\sin^3\theta}$$

Thus, one can write $x = c\cdot\cos^3\theta$, $y = c\cdot\sin^3\theta$ — c is some constant

Substitute back into $f(x,y;\theta) = 0$

$$\frac{x}{L\cos\theta} + \frac{y}{L\sin\theta} = 1 \longrightarrow \frac{c}{L}\cos^2\theta + \frac{c}{L}\sin^2\theta = 1$$

It is easy to see that $c = L$

$$\frac{x}{L} = \cos^3\theta \qquad \longrightarrow \qquad \left(\frac{x}{L}\right)^{\frac{1}{3}} = \cos\theta$$

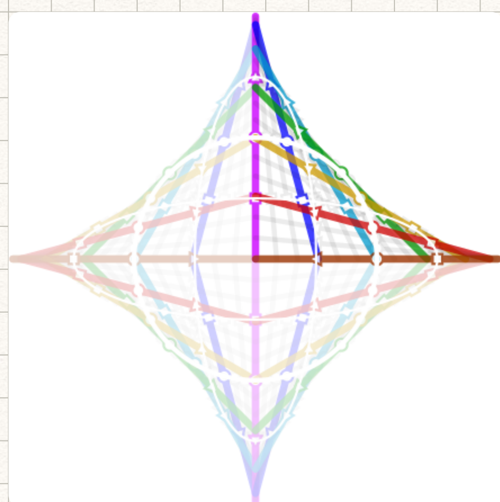
$$\frac{y}{L} = \sin^3\theta \qquad\qquad\qquad \left(\frac{y}{L}\right)^{\frac{1}{3}} = \sin\theta$$

Now we are ready to eliminate θ.

$$\frac{x}{L\cos\theta} + \frac{y}{L\sin\theta} = 1$$

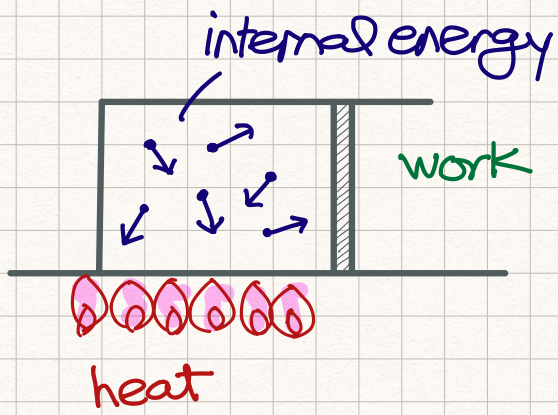
$$\frac{x/L}{(x/L)^{\frac{1}{3}}} + \frac{y/L}{(y/L)^{1/3}} = 1$$

$$\left(\frac{x}{L}\right)^{\frac{2}{3}} + \left(\frac{y}{L}\right)^{\frac{2}{3}} = 1$$



Asteroid

Thermodynamic Relations



In differential form, the 1st law of thermodynamics may be expressed as

$$dU = \underbrace{TdS}_{\text{heat}} - \underbrace{PdV}_{\text{work}}$$

Treating the internal energy $U = U(S,V)$

$$dU = \left(\frac{\partial U}{\partial S}\right)_V dS + \left(\frac{\partial U}{\partial V}\right)_S dV$$

By comparison, one can express T, P as partial derivatives of the internal energy U.

$$T = \left(\frac{\partial U}{\partial S}\right)_V , \qquad P = -\left(\frac{\partial U}{\partial V}\right)_S$$

The 2nd derivatives: $\frac{\partial^2 U}{\partial V \partial S} = \frac{\partial^2 U}{\partial S \partial V}$

$$\frac{\partial}{\partial V}\underbrace{\left(\frac{\partial U}{\partial S}\right)}_{T} = \frac{\partial}{\partial S}\underbrace{\left(\frac{\partial U}{\partial V}\right)}_{-P} \longrightarrow \underbrace{\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V}_{\text{Maxwell relation}}$$