

Grand Canonical Ensemble

①

- open systems: can exchange energy and matter with surroundings $\Rightarrow$ fix $\langle E \rangle$ and $\langle N \rangle$
- system A immersed in reservoir A' in equilibrium with each other
 - we know from thermodynamics that $T_A = T_{A'}$ and $\mu_A = \mu_{A'}$
 - N and E of system A vary

$$N_r + N_s = N^{(0)} = \text{const.}$$

$$E_s + E_r = E^{(0)} = \text{const.}$$

- reservoir is much larger than system

$$\frac{N_s}{N^{(0)}} = \left(1 - \frac{N_r}{N^{(0)}}\right) \ll 1$$

$$\frac{E_s}{E^{(0)}} = \left(1 - \frac{E_r}{E^{(0)}}\right) \ll 1$$

- the probability that the system is in state N_s, E_s is proportional to $\Omega'(N_r, E_r)$

$$P_{rs} = \Omega'(N^{(0)} - N_s, E^{(0)} - E_s)$$

expansion of $\ln P_{rs}$

$$P_{rs} = e^{\beta \mu N_r - \beta E_r}$$

~~$P_{rs} = \Omega_r$~~

normalized

$$P_{rs} = \frac{e^{\beta \mu N_r - \beta E_r}}{\sum_{rs} e^{\beta \mu N_r - \beta E_r}}$$

independent of reservoir

- some things can be shown based on ensemble theory

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$$\sum_{rs} n_{rs} = \bar{N} \quad \text{fix}$$

$$\sum_{rs} n_{rs} E_{rs} = \bar{E} \quad \text{fix}$$

number of configurations: $W(\{n_{rs}\}) = \frac{N!}{n_1! \dots n_g!}$

$$= \frac{N!}{\prod_{rs} n_{rs}!}$$

most probable configuration

$$\frac{n_{rs}}{N} = \frac{\exp[-\alpha N_{rs} - \beta E_{rs}]}{\sum_{rs} \exp[-\alpha N_{rs} - \beta E_{rs}]}$$

define: $\tilde{Q} = \sum_{rs} \exp[-\alpha N_{rs} - \beta E_{rs}]$

$$\bar{N} = -\frac{\partial \ln \tilde{Q}}{\partial \alpha} \quad \bar{E} = -\frac{\partial \ln \tilde{Q}}{\partial \beta}$$

- but here α, β are yet undetermined

- to determine what they mean

introduce q-potential

$$q = \ln \tilde{Q} = \ln \sum_{rs} \exp[-\alpha N_{rs} - \beta E_{rs}]$$

$$dq = \frac{\partial q}{\partial \alpha} d\alpha + \frac{\partial q}{\partial \beta} d\beta + \sum_{rs} \frac{\partial q}{\partial E_{rs}} dE_{rs}$$

$$\frac{\partial q}{\partial \alpha} = \frac{1}{\tilde{Q}} \frac{\partial \tilde{Q}}{\partial \alpha} = -\bar{N}$$

$$\frac{\partial q}{\partial \beta} = \frac{1}{\tilde{Q}} \frac{\partial \tilde{Q}}{\partial \beta} = -\bar{E}$$

$$\begin{aligned} \frac{\partial q}{\partial E_{rs}} &= \frac{1}{\tilde{Q}} \sum_{rs} \exp[-\alpha N_{rs} - \beta E_{rs}] (-\beta \delta E_{rs}) \\ &= -\beta \frac{\langle n_{rs} \rangle}{N} dE_{rs} \end{aligned}$$

$$dq = \cancel{\frac{\partial q}{\partial \alpha}} - \bar{N} d\alpha - \bar{E} d\beta - \frac{\beta}{N} \sum_{rs} \langle n_{rs} \rangle dE_{rs}$$

rearrange

$$d(q + \alpha \bar{N} + \beta \bar{E}) = \beta \left(\frac{\alpha}{\beta} d\bar{N} + d\bar{E} - \frac{1}{N} \sum_{rs} \langle \epsilon_{rs} \rangle dE_s \right) \quad (3)$$

- compare with first law of thermodynamics

$$\delta Q = d\bar{E} + \delta W - \mu d\bar{N} = T dS$$

associations:

$$d\bar{E} = d\bar{E}$$

$$\beta \delta Q = d(q + \alpha \bar{N} + \beta \bar{E})$$

$$\beta = 1/k_B T$$

$$\alpha = -\mu/k_B T$$

$$\delta W = -\frac{1}{N} \sum_{rs} \langle \epsilon_{rs} \rangle dE_s$$

associate

$$\frac{J}{N} = q + \alpha \bar{N} + \beta \bar{E}$$

$$\Rightarrow q = \frac{TS + \mu N - E}{kT}$$

since $\mu N = \bar{E} - TS + PV$ (Gibbs free energy)

$$q = \frac{PV}{kT}$$

$$kT \ln \left[\sum_{rs} e^{-\beta E_s + \alpha \mu N_r} \right] = PV$$

$$kT \ln \tilde{Q} = PV$$

- implied by: $Z = e^{\frac{\mu N}{kT}}$

$$q = kT \ln \left[\sum_{rs} Z^{N_r} e^{-\beta E_s} \right]$$

$$= \ln \left[\sum_r Z^{N_r} \left(\sum_s e^{-\beta E_s} \right) \right]$$

$$= \ln \left[\sum_r Z^{N_r} \underbrace{Q(N_r, T, V)}_{\text{canonical partition function } N_r, T, V} \right]$$

canonical partition function N_r, T, V

- the grand-canonical partition function is a sum over canonical partition functions

- not so surprising: the canonical partition function is a sum over microcanonical partition functions

- which one is more useful? Sometimes one sometimes the other (4)

- can obtain thermodynamics from grand canonical as well

$$PV = kT \ln \tilde{Q}(\mu, V, T)$$

$$\Rightarrow P = \frac{kT \ln \tilde{Q}(\mu, V, T)}{V}$$

$$N = \mu \frac{\partial}{\partial \mu} \ln \tilde{Q}(\mu, V, T) = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln \tilde{Q}(\mu, V, T)$$

$$U(\mu, V, T) = - \frac{\partial}{\partial \beta} \ln \tilde{Q}(\mu, V, T)$$

$$A = N\mu - PV = -kT \ln \frac{\tilde{Q}(\mu, V, T)}{\mu^N}$$

$$S = \frac{U - A}{T} = kT \frac{\partial \ln \tilde{Q}}{\partial T} - N \ln \mu + k \ln \tilde{Q}$$

~~$$\frac{\partial N}{\partial \mu} = \frac{1}{\beta} \frac{\partial^2}{\partial \mu^2} \ln \tilde{Q}(\mu, V, T) = \frac{1}{\beta} \langle N^2 \rangle - \langle N \rangle^2$$~~

↑
extensive divided by intensive $\Rightarrow$ scales as N

↓
fluctuations $\langle N^2 \rangle - \langle N \rangle^2$ scale as N

relative fluctuations $\Rightarrow \frac{\sqrt{\langle \Delta N^2 \rangle}}{\langle N \rangle} = \frac{\sqrt{\langle N^2 \rangle - \langle N \rangle^2}}{\langle N \rangle}$ scale as $\frac{1}{\sqrt{N}}$

One can also write

$$\langle N^2 \rangle - \langle N \rangle^2 = kT \frac{\partial \langle N \rangle}{\partial \mu} = \frac{k_B T \langle N \rangle^2}{V} \kappa_T$$

↑
isothermal compressibility

examples: simple problems

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- classical ideal gas

$$Q_N(V, T) = \frac{[Q_1(V, T)]^N}{N!}$$

$Q_1(V, T)$ - partition function for single particle

- $N!$ result of delocalization of particles

indistinguishability $\leftrightarrow$ delocalization

$Q_1(V, T) = V f(T)$ - proportional to volume, since the greater the volume, the greater the number of microstates available to a single particle

$$\tilde{Q}(z, V, T) = \sum_{N=0}^{\infty} \frac{z^N V^N f(T)^N}{N!} = \exp[z V f(T)]$$

$$\begin{aligned} \left\{ \begin{aligned} P &= z k T f(T) \left(= \frac{k T \ln \tilde{Q}}{V} \right) \\ N &= z V f(T) = z \frac{\partial}{\partial z} \ln \tilde{Q} \\ U &= z V k T^2 f'(T) = - \frac{\partial \ln \tilde{Q}}{\partial \beta} = k T^2 \frac{\partial \ln \tilde{Q}}{\partial T} \end{aligned} \right. \quad \begin{aligned} z &= e^{\beta \mu} \\ \ln z &= \beta \mu \end{aligned}$$
$$A = N \mu - P V = N k T \ln z - k T \ln \tilde{Q}$$
$$= N k T \ln z - k T z V f(T)$$
$$S = \frac{U - A}{T} = z V k T f'(T) - N k \ln z + k z V f(T)$$

$\rightarrow PV = N k T$ irrespective of $f(T)$

$\rightarrow U = N k T^2 f'(T) / f(T)$

Suppose $f(T) = A T^n \Rightarrow U = n N k T$

- one can also eliminate z so that 1

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- second example: consider independent, localized particles

- here microscopic entities are mutually distinguishable

$$Q_N(V, T) = [Q_1(V, T)]^N$$

- in this case $Q_1(V, T) = \phi(T)$ (independent of volume)

$$\tilde{Q}(z, V, T) = \sum_{N=0}^{\infty} z^N \phi(T)^N = [1 - z\phi(T)]^{-1}$$

$z\phi(T) < 1$ for convergence

thermodynamics follows from $kT \ln \tilde{Q} = PV$

$$P = \frac{kT \ln \tilde{Q}}{V} \quad \text{in this case as } V \rightarrow \infty$$

T intensive
so $P=0$

$$N = z \frac{\partial}{\partial z} kT \ln \tilde{Q} = kT \frac{1}{\tilde{Q}} \frac{\partial \tilde{Q}}{\partial z} = \frac{kT z \phi(T)}{[1 - z\phi(T)]^2}$$

$$= \frac{z \phi(T)}{[1 - z\phi(T)]}$$

$$U = - \frac{\partial}{\partial \beta} kT \ln \tilde{Q} = - \frac{\partial \ln \tilde{Q}}{\partial T} \frac{\partial T}{\partial \beta} = kT^2 \frac{\partial \ln \tilde{Q}}{\partial T} =$$

$$= \frac{-kT^2 [-z\phi'(T)]}{[1 - z\phi(T)]} = \frac{kT^2 z\phi'(T)}{1 - z\phi(T)}$$

$$A = N\mu - PV = NkT \ln z + kT \ln [1 - z\phi(T)]$$

$$S = -Nk \ln z - k \ln [1 - z\phi(T)] + \frac{2kT\phi'(T)}{1 - z\phi(T)}$$

$\rightarrow z\phi(T) = \frac{N}{N+1} \approx 1 - \frac{1}{N} \quad N \gg 1$

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$$\Rightarrow \frac{U}{N} = \frac{kT^2 \phi'(T)}{\phi(T)}$$

$$\frac{A}{N} = -kT \ln \phi(T) + O\left(\frac{\ln N}{N}\right)$$

$$\frac{S}{N} = \ln \phi(T) + T \frac{\phi'(T)}{\phi(T)} + O\left(\frac{\ln N}{N}\right)$$

for quantum harmonic oscillators $\phi(T) = \left[2\pi m h \left(\frac{g\omega}{hT} \right) \right]^{-1}$

for classical harmonic oscillators $\phi(T) = \frac{kT}{h\omega}$

solid-vapor equilibrium

- consider ~~box~~ containing solid and vapor

- closed vessel at T, V

- mutual equilibrium $\mu_s = \mu_g$ (they are free to exchange particles)

$$\Downarrow$$

$$Z_s = Z_g$$

$$\text{for gas: } Z_g = \frac{N_g}{V_g \phi(T)}$$

$N_g \sim$ number of gas particles

$V_g \sim V$ (typically)

$$Z_s \approx \frac{1}{\phi(T)} \quad \text{since } Z_g(T) \approx 1 - \frac{1}{N}$$

$$\text{since } Z_s = Z_g \Rightarrow \frac{N_g}{V_g} = \frac{\phi(T)}{\phi(T)}$$

- at high temperatures, at low vapor densities $[PV = NkT]$

$$\Rightarrow P_{\text{vapor}} = \frac{N_g}{V_g} kT = kT \frac{\phi(T)}{\phi(T)}$$

$$S(T) = \frac{(2\pi m kT)^{3/2}}{h^3}$$

$$\phi(T) = \left[2\pi \sinh\left(\frac{h\omega}{2kT}\right) \right]^{-3}$$

$$P_{\text{gas}} = kT \left(\frac{2\pi m kT}{h^2} \right)^{3/2} \left[2 \sinh \left(\frac{q_w}{2kT} \right) \right]^3 e^{-\epsilon/kT}$$

⑧

ϵ - energy to ~~localize~~ ^{delocalize} a particle

- condition to form solid phase

$$N > V \frac{s(T)}{d(T)} \quad \left[\begin{array}{l} N > N_g \\ V \approx V_g \end{array} \right]$$

- One there are two phases

$$\Rightarrow \frac{N_g(T)}{V} = \frac{s(T)}{d(T)}$$

$N_g(T)$ - gas atoms

$N_s(T) = N - N_g(T)$ - solid atoms

Fluctuations in grand canonical ensemble

- relative fluctuations are negligible

$$\overline{N^2} - \overline{N}^2 = kT \frac{\partial \overline{N}}{\partial \mu}$$

- relative fluctuation in particle densities $n = \overline{N}/V$

$$\frac{\overline{\Delta N^2}}{\overline{N}^2} = \frac{\overline{\Delta n^2}}{\overline{n}^2} = \frac{kT}{\overline{N}^2} \left(\frac{\partial \overline{N}}{\partial \mu} \right)_{T,V} \quad v = V/\overline{N}$$

$$= \frac{kT v^2}{V^2} \left(\frac{\partial (V/v)}{\partial \mu} \right)_{T,V} = - \frac{kT}{V} \left(\frac{\partial v}{\partial \mu} \right)_T$$

- can recast using thermodynamic relations

$$d\mu = v dp - s dT \quad v = \frac{V}{N} \quad s = \frac{S}{N}$$

$$\left(\frac{\partial \mu}{\partial p} \right)_T = v \quad \left(\frac{\partial v}{\partial \mu} \right)_T \left(\frac{\partial \mu}{\partial p} \right)_T = \left(\frac{\partial v}{\partial p} \right)_T = \left(\frac{\partial v}{\partial p} \right)_T$$

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$$\Rightarrow \overline{\frac{\Delta n^2}{n^2}} = -\frac{nT}{V} \left(\frac{\partial V}{\partial P} \right)_T = \frac{nT}{V} \kappa_T$$

κ_T - isothermal compressibility

- fluctuations are usually negligible $\frac{\Delta n^2}{N} \sim \frac{1}{N^{1/2}}$ as $N \rightarrow \infty$

- exceptions: phase transitions

$\Rightarrow$ compressibility at critical point often

diverges $\Rightarrow$ correlations diverge

- for example: both compressibility and rootmean square fluctuations scale with N to some power at critical point

in such cases: canonical and grand canonical do not give the same results

$\Rightarrow$ grand canonical to be preferred

energy fluctuations:

$$\overline{\Delta E^2} = \overline{E^2} - \bar{E}^2 = - \left(\frac{\partial \bar{E}}{\partial \beta} \right)_{T,V} = kT^2 \left(\frac{\partial U}{\partial T} \right)_{T,V}$$

$$\left(\frac{\partial U}{\partial T} \right)_{T,V} = \left(\frac{\partial U}{\partial T} \right)_{N,V} + \left(\frac{\partial U}{\partial N} \right)_{T,V} \left(\frac{\partial N}{\partial T} \right)_{T,V}$$

$$N = - \partial_\alpha \ln \tilde{Q} \quad E = - \partial_\beta \ln \tilde{Q}$$

$$\left(\frac{\partial N}{\partial \beta} \right)_{T,V} = \left(\frac{\partial U}{\partial \alpha} \right)_{T,V}$$

$$\left(\frac{\partial N}{\partial T} \right)_{T,V} = \frac{1}{T} \left(\frac{\partial U}{\partial N} \right)_{T,V}$$

$$\Delta E^2 = kT^2 C_V + kT^2 \left(\frac{\partial U}{\partial N} \right)_{T,V} \frac{1}{T} \left(\frac{\partial U}{\partial T} \right)_{T,V}$$

$$= kT^2 C_V + \left(\frac{\partial U}{\partial N} \right)_{T,V} + kT^2 \left(\frac{\partial U}{\partial N} \right)_{T,V} \frac{1}{T} \left(\frac{\partial U}{\partial T} \right)_{T,V}$$

$$= kT^2 C_v + kT \left(\frac{\partial U}{\partial N} \right)_{T,V} \left(\frac{\partial U}{\partial N} \right)_{T,V} \left(\frac{\partial N}{\partial \mu} \right)_{T,V}$$

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$$= kT^2 C_v + kT \left[\left(\frac{\partial U}{\partial N} \right)_{T,V} \right]^2 (\overline{N^2} - \overline{N}^2)$$

energies fluctuations ~~are~~ include the same terms as for the canonical ensemble + term due to particle fluctuations

- for phase transitions these fluctuations are present $\Rightarrow$ need to be included $\Rightarrow$ more appropriate to use grand-canonical formalism

Probability theory

- ensemble theory: for systems with a large number of variables
"ensemble" or probabilistic description is necessary
- stochastic variables: value is the outcome of an experiment
- most we can know: particular value will be realized in an experiment

Permutations and Combinations

- two principles for counting problems

a) addition principle: if two operations are mutually exclusive, and the first can be done in m ways and the second can be done in n ways, then

one or the other can be done in $m+n$ ways

b) multiplication principle: if an operation can be performed in m ways, and another operation can be performed in n ways, then the two operations can be performed in $m \cdot n$ ways

- two underlying principles

permutation or combination

permutation: is an arrangement of some number of objects in a definite order

N objects: $N!$ distinct permutations

if we have N objects and we take R objects from those N objects

$\Rightarrow$ number of distinct combinations $\frac{N!}{(N-R)!}$

$$P_R^N = \frac{N!}{(N-R)!}$$

- combination: selection of N distinct objects without regard to order

number of combinations of R objects taken from

$$N \text{ objects: } C_N^R = \frac{N!}{R!(N-R)!} = \frac{P_N^R}{R!}$$

number of distinct permutations of R objects
~~to~~ selected from N objects divided
 by number of distinct permutations
 of R -objects

- probability: quantization of our expectation of an event

- suppose an outcome of an experiment is A

then if N experiments are performed

then the number of experiments with
 outcome A is $NP(A)$ [$N \rightarrow \infty$]

- sample space: S - ~~infinite~~ set which includes all outcomes of
 a particular event/experiment

- to find probability of an event A

- set up sample space of all ~~events~~ possible
 outcomes $\Rightarrow S$

- assign probabilities to each element of
 sample space

- to obtain probability of A , add probabilities
 assigned to sample space for those outcomes
 which are consistent with outcome A

- set theory: union of two events: $A \cup B$
- set of all points belonging to A and/or B

intersection of two events: $A \cap B$

- set of all points belonging to both
 A and B

if A and B are mutually exclusive $A \cap B = \emptyset$
 $\emptyset$ empty set

let $P(A)$ denote the probability for outcome A

let $P(\emptyset) = 0$ $P(S) = 1$

then

$$P(A \cup B) = P(A) + P(B) - P(A \cap B)$$

$P(A)$ includes $P(A \cap B)$ $\rightarrow P(A \cap B)$ is double counted
 $P(B)$ includes $P(A \cap B)$

if A and B are mutually exclusive

$$P(A \cup B) = P(A) + P(B)$$

if $A_1, \dots, A_m$ are mutually exclusive and exhaustive

$$\Rightarrow A_1 \cup A_2 \cup \dots \cup A_m = S$$

$$P(A_1) + \dots + P(A_m) = 1$$

events A and B are independent if and only if

$$P(A \cap B) = P(A)P(B)$$

independent events are not mutually exclusive

$P(A \cap B) = 0$ for mutually exclusive events

conditional probability: $P(B|A)$ - probability that A occurs given that B occurred

$$P(B|A) = \frac{P(A \cap B)}{P(A)} \Rightarrow P(A)P(B|A) = P(A \cap B)$$

if A and B are independent $\Rightarrow P(B|A) = P(B)$

stochastic variable: quantity whose value is determined by the outcome of an experiment

stochastic variable X on sample space S maps elements

S into a set of real numbers $\mathbb{R}$

stochastic variable X , possible realizations: $x_1, \dots, x_n$

distribution functions

- discrete stochastic variables

- let X be a stochastic variable on sample space S

with a countable set of realizations $\{x_i\}$ $i=1, \dots, n$

(n = finite or ∞)

- assign probability p_i to each x_i

$$p_i \geq 0 \quad \sum p_i = 1$$

- probability density function

$$P_X(x) = \sum_{i=1}^n p_i \delta(x - x_i)$$

- (cumulative) distribution function

$$F_X(x) = \int_{-\infty}^x P_X(x) dx$$

$$= \sum_{i=1}^n p_i \Theta(x - x_i)$$

$\Theta(x - x_i)$ - Heaviside function

$$P_X(x) = \frac{dF_X(x)}{dx}$$

$F_X(x)$ - probability that stochastic variable falls in interval $(-\infty, x)$

$F_X(x)$ - monotonically increasing,

since $P_X(x) \geq 0$

$$F_X(-\infty) = 0$$

$$F_X(\infty) = 1$$

Continuous Stochastic Variables

let X be a stochastic variable which can take on a continuous set of values

Prob event in this case: $a \leq x \leq b$

$P_X(x)$ - piecewise continuous function

s.t. the probability that X has

a value in the interval $a \leq x \leq b$

is given by the area under the curve

$$P(a \leq x \leq b) = \int_a^b dx P_X(x)$$

$\Downarrow$ $\Downarrow$
 $P_X(x)$ - probability for a stochastic variable

$$P_X(x) \geq 0 \quad \int P_X(x) dx = 1$$

can also define (cumulative) distribution function

$$F_X(x) = \int_{-\infty}^x dy P_X(y)$$

$$F_X(-\infty) = 0$$

$$F_X(\infty) = 1 \text{ monotonically increasing}$$

to switch between two stochastic variables

$\Rightarrow$ let $Y = H(X)$ X - stochastic variable
 Y - stochastic variable

$$P_Y(y) = \int_{-\infty}^{\infty} dx \delta(y - H(x)) P(x)$$

Moments

- if we know $P_X(x)$ for a stochastic variable
 - $\Rightarrow$ we know everything about it
- we do not always know $P_X(x)$
 - one way is to reconstruct it from its moments

moment of distribution:

$$\langle x^n \rangle = \int_{-\infty}^{\infty} dx x^n P(x)$$

variance: $\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$

1st moment:

$\langle x \rangle$ — "center of mass" of distribution

! not to be confused with most probable x value (x_p)

nor with median x -value (x_m)

- median: value of x which divides the curve into parts with equal area

$$F_X(x_m) = \frac{1}{2}$$

2nd moment

$\langle x^2 \rangle$ gives information about spread around $x=0$ or mean if we consider

$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$$

3rd moment

$\langle x^3 \rangle$ — info about "skewness" of distribution about $x=0$

Characteristic functions

$$f_X(k) = \langle e^{ikx} \rangle = \int_{-\infty}^{\infty} dx e^{ikx} P_X(x) = \sum_{n=0}^{\infty} \frac{(ik)^n \langle x^n \rangle}{n!}$$

- meaningful if series converges
- to determine probability density one needs all moments
- $f_X(k)$ continuous; $f_X(0) = 1$, $|f_X(k)| \leq 1$
 $f_X(k) = f_X^*(-k)$

$$P_X(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk f_X(k) \quad \text{inverse FT of characteristic function gives } P_X(x)$$

moments from characteristic function

$$\langle x^n \rangle = \lim_{k \rightarrow 0} (-i)^n \frac{d^n f_X(k)}{dk^n}$$

cumulants:

$$f_X(k) = \exp \left(\sum_{n=1}^{\infty} \frac{(ik)^n}{n!} C_n(x) \right)$$

to obtain cumulants: expand exponential, compare with $\sum_{n=0}^{\infty} \frac{(ik)^n \langle x^n \rangle}{n!}$, and equate equal powers of k .

$$1 + \sum_{n=1}^{\infty} \frac{(ik)^n}{n!} C_n(x) + \frac{1}{2} \left[\sum_{n=1}^{\infty} \frac{(ik)^n}{n!} C_n(x) \right]^2 + \dots$$
$$= \frac{(ik) \langle x \rangle}{1} + \frac{(ik)^2 \langle x^2 \rangle}{2}$$

$$1 + \frac{(ik)}{1} C_1(x) + \frac{(ik)^2}{2} C_2(x) + \frac{1}{2} \frac{(ik)^2}{1 \cdot 1} C_1(x) C_1(x) + \dots$$

$$\rightarrow C_1(x) = \langle x \rangle$$

$$C_2(x) = \langle x^2 \rangle - \langle x \rangle^2$$

$$\text{Similarly, } \rightarrow C_3(x) = \langle x^3 \rangle - 3\langle x \rangle \langle x^2 \rangle + 2\langle x \rangle^3 \dots$$

- using cumulants we can reconstruct characteristic function $\Rightarrow$ distribution
- especially if they go to zero rapidly as a function of n

of n

jointly distributed stochastic variables

stochastic variables: $X_1, X_2, \dots, X_n$ jointly distributed if defined on same sample space S

$$F_{X_1, \dots, X_n}(x_1, \dots, x_n) \equiv \text{Prob}\{X_1 < x_1, \dots, X_n < x_n\}$$

$$\{X_1 < x_1, \dots, X_n < x_n\} = \{X_1 < x_1\} \cap \dots \cap \{X_n < x_n\}$$

from F (cumulative) distribution function

$\Rightarrow$ one can obtain $P(x_1, \dots, x_n)$

$$P(x_1, \dots, x_n) = \frac{\partial^n F_{X_1, \dots, X_n}(x_1, \dots, x_n)}{\partial x_1 \dots \partial x_n}$$

$$F_{X_1, \dots, X_n}(x_1, \dots, x_n) = \int_{-\infty}^{x_1} \dots \int_{-\infty}^{x_n} d x_1 \dots d x_n P_{X_1, \dots, X_n}(x_1, \dots, x_n)$$

- two variable joint distribution

$$P_{X,Y}(x,y) : F_{X,Y}(-\infty, y) = F_{X,Y}(x, -\infty) = F_{X,Y}(\infty, \infty) = 0$$

$$F_{X,Y}(\infty, \infty) = 1$$

$$\text{also } F_{X,Y}(x_2, y) - F_{X,Y}(x_1, y) = \text{Prob}\{x_1 \leq X \leq x_2; Y \leq y\} \geq 0$$

$x_2 > x_1$

- normalisation : $\int dx dy P_{X,Y}(x,y) = 1$

reduced distribution function

$$F_x(x) = F_{x,y}(x, \infty) = \int_{-\infty}^x dx' \int_{-\infty}^{\infty} dy' P_{xy}(x', y')$$

reduced probability densities

$$P_x(x) = \int_{-\infty}^{\infty} dy P_{xy}(x, y)$$

nth moment: $\langle x^n \rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy x^n P_{xy}(x, y)$

joint moments: $\langle x^n y^m \rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy x^n y^m P_{xy}(x, y)$

covariance: $\text{Cov}(X, Y) = \langle (x - \langle x \rangle)(y - \langle y \rangle) \rangle$
 $= \langle xy \rangle - \langle x \rangle \langle y \rangle$

correlation function:

$$\text{Cor}(X, Y) = \frac{\langle (x - \langle x \rangle)(y - \langle y \rangle) \rangle}{\sigma_x \sigma_y}$$

- measure of the degree of dependence
of variables x, y

properties of correlation function

- (i) $\text{Cor}(X, Y) = \text{Cor}(Y, X)$
- (ii) $-1 \leq \text{Cor}(X, Y) \leq 1$
- (iii) $\text{Cor}(X, X) = 1$ $\text{Cor}(Y, -X) = -1$
- (iv) $\text{Cor}(aX + b, cY + d) = \text{Cor}(X, Y)$
 $a, c \neq 0$

idea can be extended to any number of variables

for independent variables

$$P_{x,y}(x, y) = P_x(x) P_y(y)$$

$$\langle xy \rangle = \langle x \rangle \langle y \rangle$$

$$\text{Cor}(X, Y) = 0$$

the converse does not necessarily hold

- independent variables are always uncorrelated

- uncorrelated variables are not always independent

- suppose $Z = G(X, Y)$

if X, Y are stochastic variables $\Rightarrow \Rightarrow$ is Z

its probability distribution is given by

$$P_Z(z) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \delta(z - G(x, y)) P_{X,Y}(x, y)$$

characteristic function

$$\begin{aligned} f_Z(k) &= \int dz e^{ikz} P_Z(z) \\ &= \int_{-\infty}^{\infty} dx dy e^{ikG(x, y)} P_{X,Y}(x, y) \end{aligned}$$

- characteristic functions of jointly distributed variables

$$f_{X_1 \dots X_n}(k_1 \dots k_n) = \int_{-\infty}^{\infty} dx_1 \dots dx_n e^{i(k_1 x_1 + \dots + k_n x_n)} P_{X_1 \dots X_n}(x_1 \dots x_n)$$

$$\langle X_1^{m_1} \dots X_n^{m_n} \rangle = \lim_{k_1 \rightarrow 0} \dots \lim_{k_n \rightarrow 0} \frac{\partial}{\partial k_1} \dots \frac{\partial}{\partial k_n} f_{X_1 \dots X_n}(k_1 \dots k_n)$$