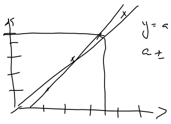
Lineær regresjon

- hånd
- kalkulator - standardavvik
- Matlab / Python



$y = ax + b$

$a \pm \sigma_a$

$x = 2, 4, 6, 8, 10$

$y = 8, 12, 34, 56, 110$

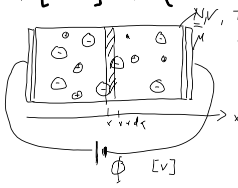
$y = bx^2$, $y = bx + cx^2$, $\underline{y = a + bx + cx^2}$

$y = \mathbb{X} b$ $\quad \mathbb{X} = x^2$ $\quad X = [\cancel{x} \; x^2]$ $\quad X = [1 \;\; x \;\; x^2]$

Li-ione-batterier

Spenning over cellen

=> hva slags fordeling $n(x)$ får vi i likevekt?



+ ioner bevegelige
- ioner sitter fast
* ionkonsentrasjon n_0 liten
=> + ionene vekselvirker ikke

kjemisk likevekt

kjemisk potensial $\mu = \mu_{indre} + \mu_{elekt}$

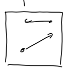
~~Ka~~ Modell: ideell gass

—— || —— til eksternt felt $\mu_{elekt} = \varphi \cdot q$

/ Poissons ligning $\nabla^2 \varphi = -\frac{\rho}{\varepsilon}$)

Kjemisk pot. ideell gass. monatomisk

(NPT) (NVT)
(NVE) (NPS)



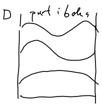
N, V, T

$Z_N = \frac{1}{N!} Z_1^N$

$Z_1 =$ Boltzmannsummen over alle tilstander s, E(s)

$= \sum e^{-E(s)/kT} = \sum_n e^{-E_n/kT}$

1D partikkel i boks



$\lambda_3 = \frac{2L}{3}$

$\lambda_2 = \frac{2L}{2}$

$\lambda_1 = 2L$

$\lambda_n = \frac{2L}{n}$ $\quad E_n = \frac{p_n^2}{2m} = \frac{1}{2}mv^2$

$p_n = \frac{h}{\lambda_n} = \frac{hn}{2L}$

$E_n = \frac{h^2 n^2}{8mL^2}$

1D tilstandssum: $Z_{1,1D} = \sum e^{-\frac{h^2n^2}{8mL^2}/kT}$

h liten $\quad = \int_0^\infty e^{-\frac{h^2n^2}{8mL^2 kT}} dn = \frac{L}{l_Q}$ $\quad l_Q = \frac{h}{\sqrt{2\pi m kT}}$

3D $\quad Z_{1,3D} = \frac{L_x}{l_Q}\frac{L_y}{l_Q}\frac{L_z}{l_Q} = \frac{V}{v_Q}$ $\quad v_Q = \frac{h^3}{(2\pi m kT)^{3/2}}$

$Z_N = \frac{1}{N!}(Z_{1,3D})^N = \frac{1}{N!}\left(\frac{V}{v_Q}\right)^N$ $\quad \underline{\frac{V}{v_Q} = n_Q}$

Stirling: $\ln N! = \underline{N(\ln N - 1)} + O(\ln N)$

$$\underline{\ln Z_N = N[\ln V - \ln v_Q - \ln N + 1]}$$

Ideell gass $\quad = N[\ln n_Q - \ln N + 1]$

NVT: $\underline{F = U - TS}$ Helmholtz

Generelt $\quad -S = \frac{F-U}{T} = \left(\frac{\partial F}{\partial T}\right)_{V,N}$

Finner vi F finner vi alt:

$P = -\left(\frac{\partial F}{\partial V}\right)_{T,N}$

$S = -\left(\frac{\partial F}{\partial T}\right)_{V,N}$

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

$\boxed{F = -kT \ln Z}$ løsn?

$\frac{\partial F}{\partial T} = -k \ln Z - kT \frac{\partial \ln Z}{\partial T}$

$\beta = \frac{1}{kT}$ $\quad \frac{\partial}{\partial T} \ln Z = \frac{\partial \beta}{\partial T}\frac{\partial \ln Z}{\partial \beta} = -\frac{1}{kT^2}\frac{1}{Z}\frac{\partial Z}{\partial \beta}$

Fra før $\quad U = \bar{E} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta}$

$\frac{\partial \ln Z}{\partial T} = \frac{U}{kT^2}$

$\frac{\partial F}{\partial T} = \underbrace{-k \ln Z}_{\frac{F}{T}} - \underbrace{\cancel{kT}\frac{U}{\cancel{k}T^2}}_{\frac{U}{T}} = \frac{F-U}{T}$ $\quad$ Én løsning

Tester for $\underline{T=0}$ $\quad F(T=0) = \underline{U_0} = -kT \ln e^{-U_0/kT} = \underline{U_0}$ eneste løsn.

$$\boxed{F = -kT \ln Z}$$

Kjemisk pot. $\quad \mu = \left(\frac{\partial F}{\partial N}\right)_{V,T}$

Ideell gass
$Z = N[\ln n_Q - \ln N + 1]$

$\left(\frac{\partial F}{\partial N}\right)_{V,T} = -kT[\ln n_Q - \ln N + 1] + kT\left(N\frac{1}{N}\right)$!

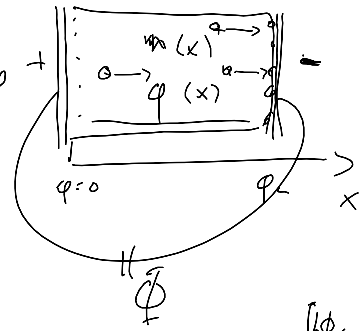
$= -kT \ln \frac{n_Q}{N} = kT \ln \frac{N}{n_Q}$

$$\boxed{\mu = kT \ln \frac{N}{n_Q}}$$

Batteri

$$\mu_{tot} = \mu_{int} + \mu_{ext} = kT \ln \frac{n}{n_Q} + q\varphi$$

$$= kT \ln \frac{n(x)}{n_Q} + q\varphi$$



Likevekt? $\mu_{tot}(x) = \text{konst}$

$$\mu_{tot}(x=0) = \mu_{tot}(x=L)$$

$$kT \ln \frac{n(0)}{n_Q} = kT \ln \frac{n(L)}{n_Q} + q\phi_L$$

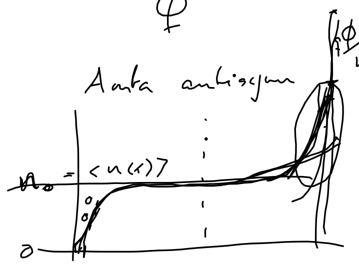
$$\frac{n(0)}{n(L)} = e^{q\phi_L/kT}$$

$$n_0 - n(0) = -(n_0 - n(L))$$

$$2n_0 = n(0) + n(L)$$

$$= n(L)\left(1 + e^{q\phi_L/kT}\right)$$

Anta antisymm



$$\Rightarrow \quad n(L) = \frac{2n_0}{1 + e^{q\phi/kT}}$$

$$n(0) = \frac{2n_0}{1 + e^{-q\phi/kT}}$$

$$\mu(x) = \mu_0 = kT \ln \frac{n(x)}{n_Q} + q\varphi(x)$$

$$\frac{n(x)}{n_Q} = e^{(q\varphi(x) - \mu_0)/kT}$$