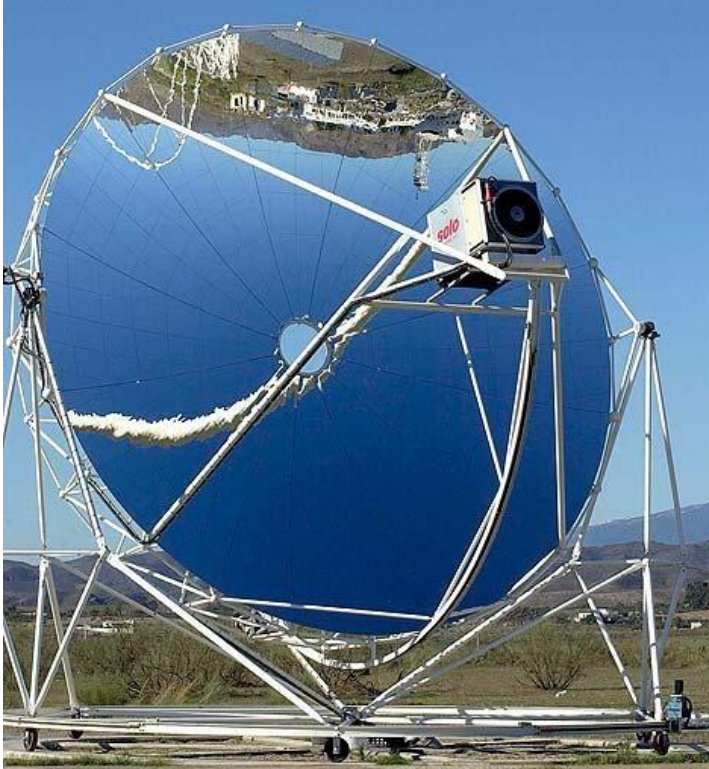


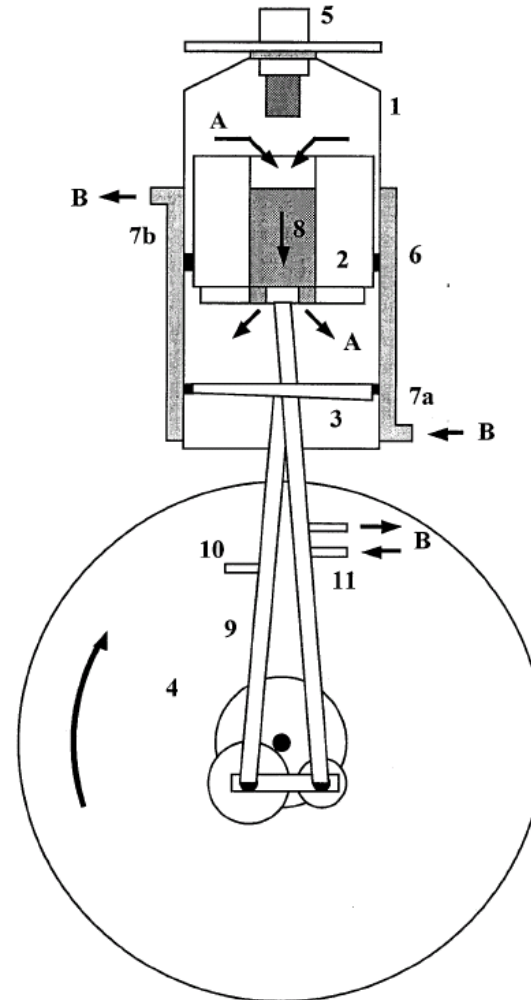
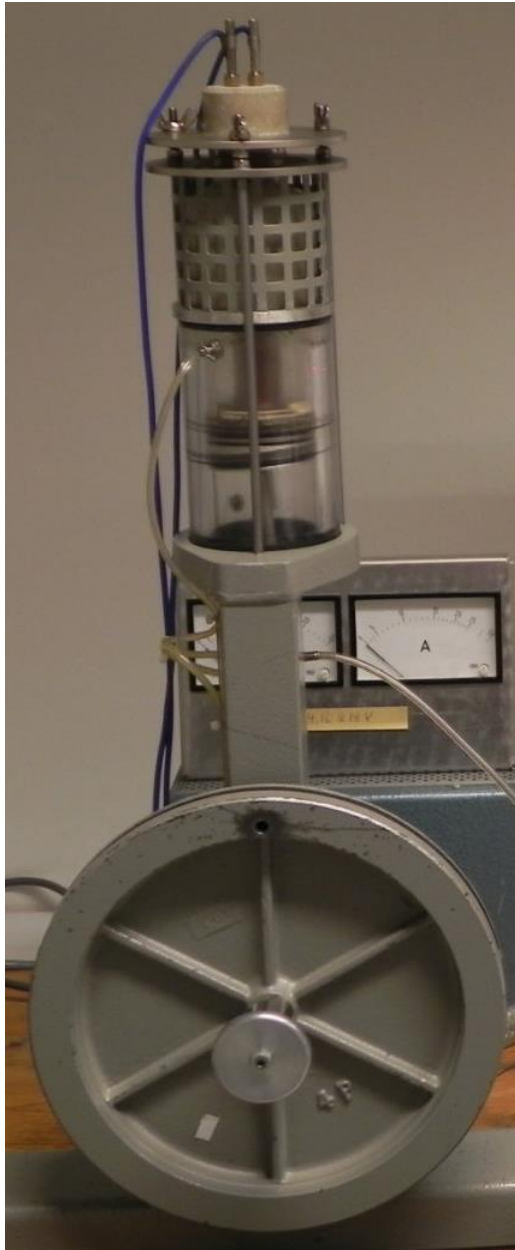
Hur omvandlas värme till elenergi i en Stirlingmotor ?



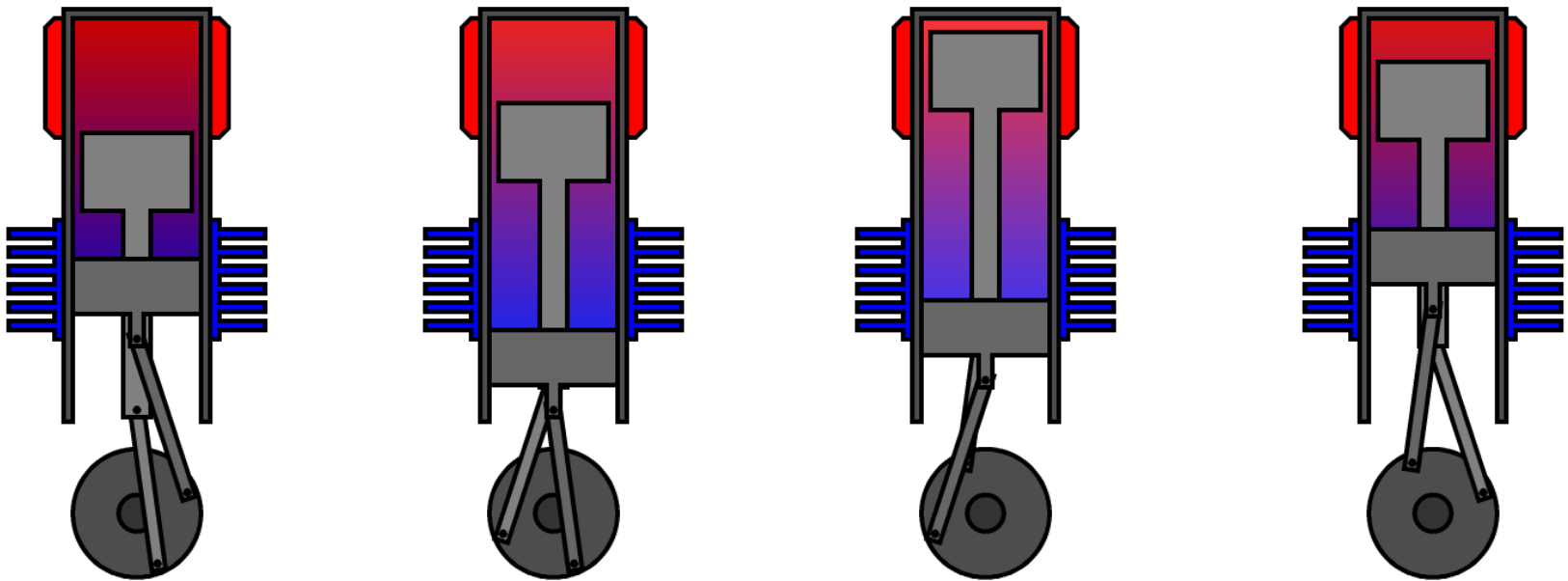
Hur fungerar kompressorkylskåpet ?



Stirlingmotorn Varmluftsmotorn

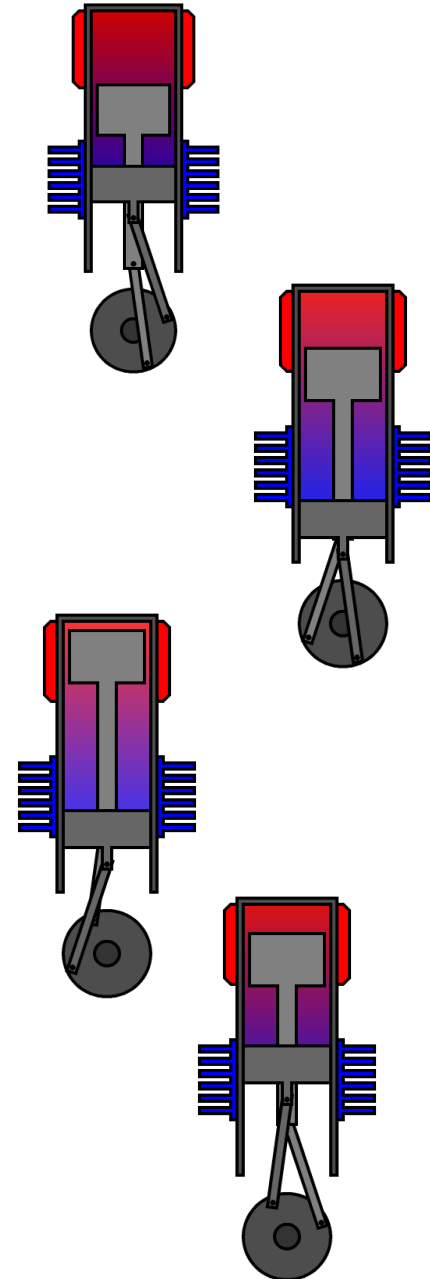


Stirlingmotorn

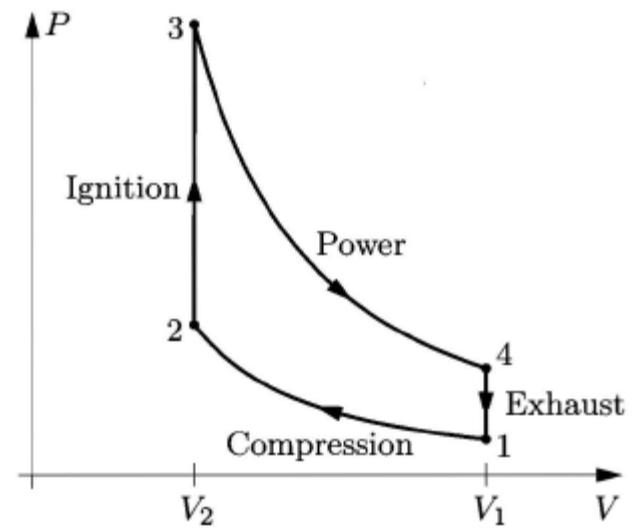
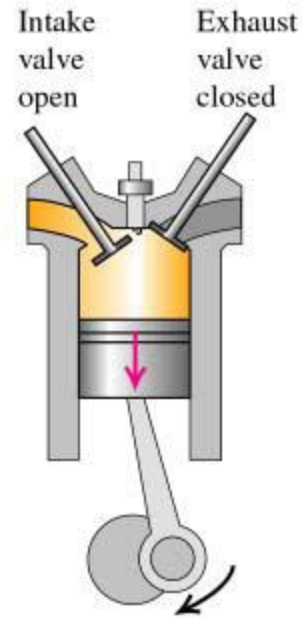


Stirlingmotorn

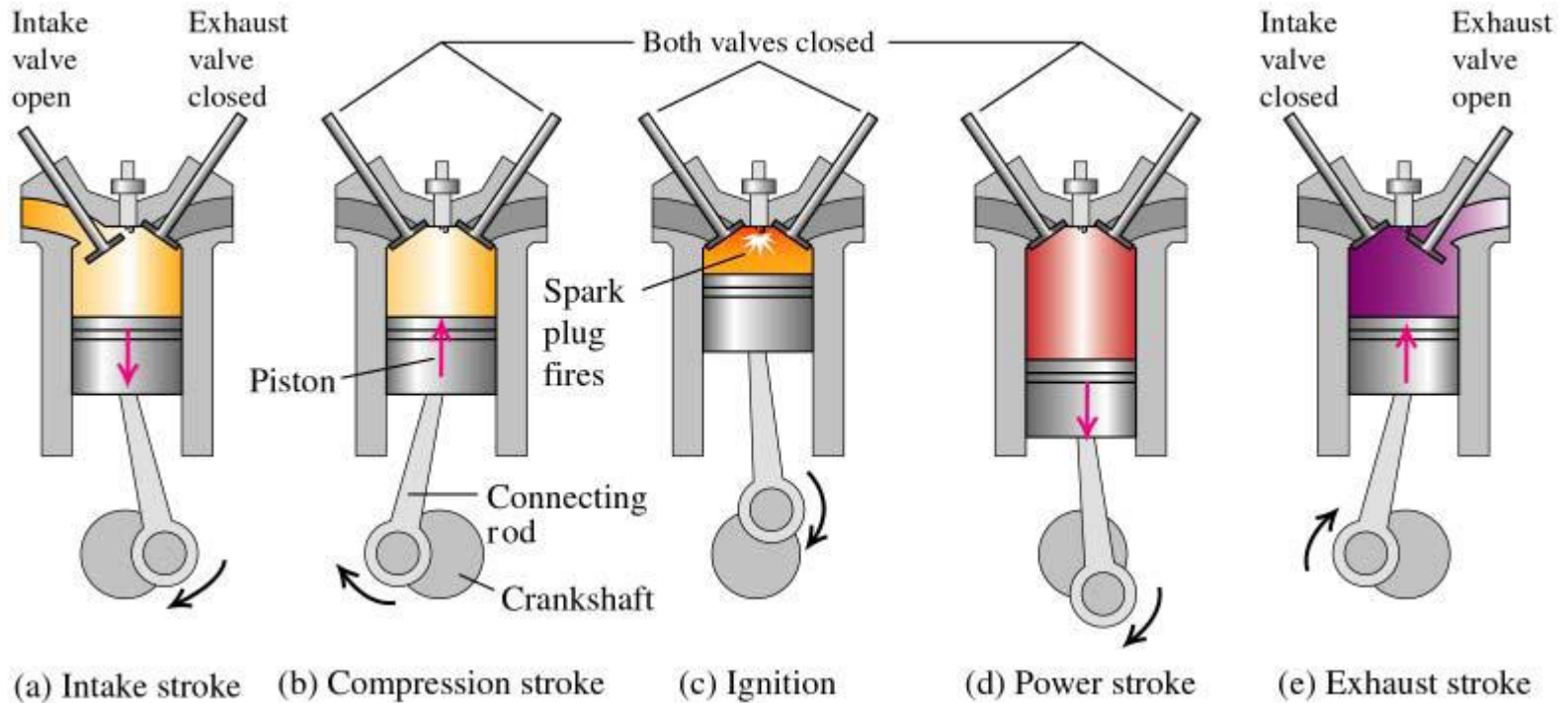
- **1.** Arbetskolven har pressat ihop (komprimerat) gasen och transportkolven har flyttat mesta gasen till cylinderns varma ändan.
- **2.** Gasen värms upp nu. Den uppvärmda gasen ökar därmed sitt tryck och pressar arbetskolven nedåt längs cylindern – här utföras arbete.
- **3.** Transportkolven flyttar nu gasen till den kalla ändan av cylindern. Värme avges.
- **4.** Gasen kyls ner samtidigt som den pressas ihop med hjälp av svänghjulets rörelse. Här tillförs arbete.



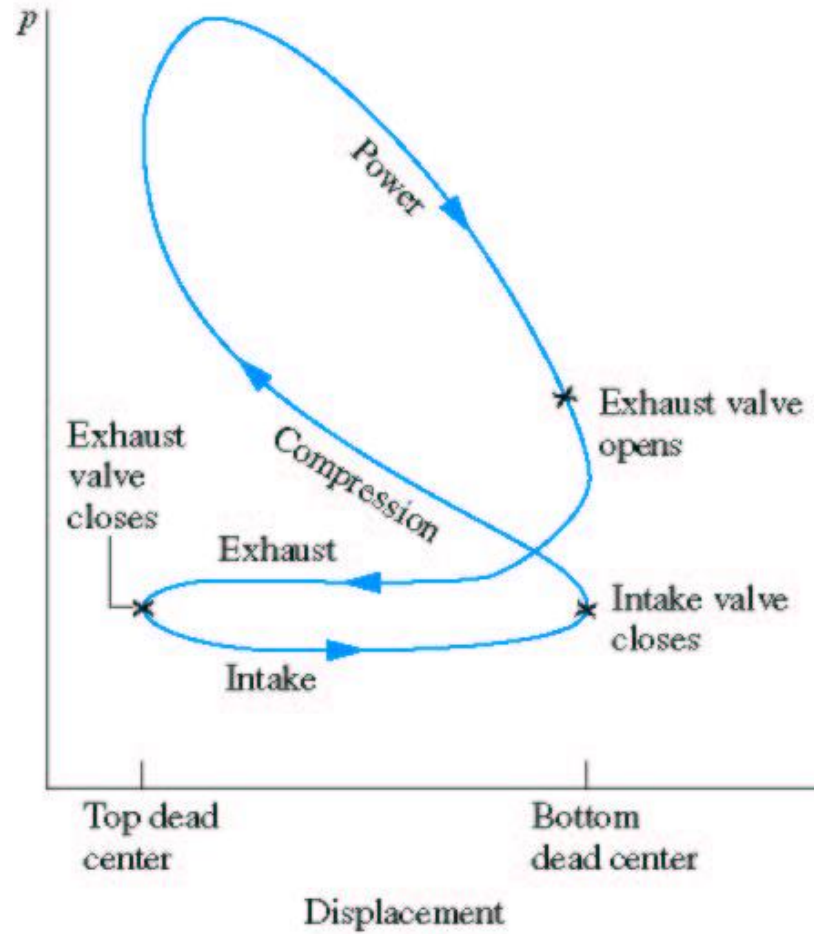
Ottomotorn



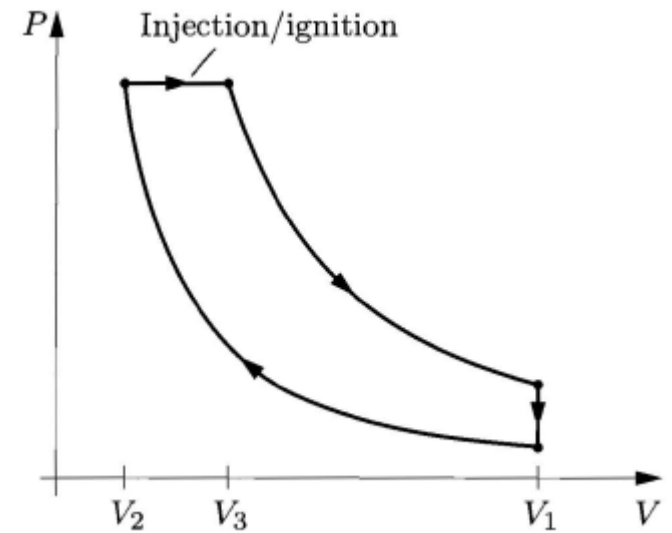
Ottomotor



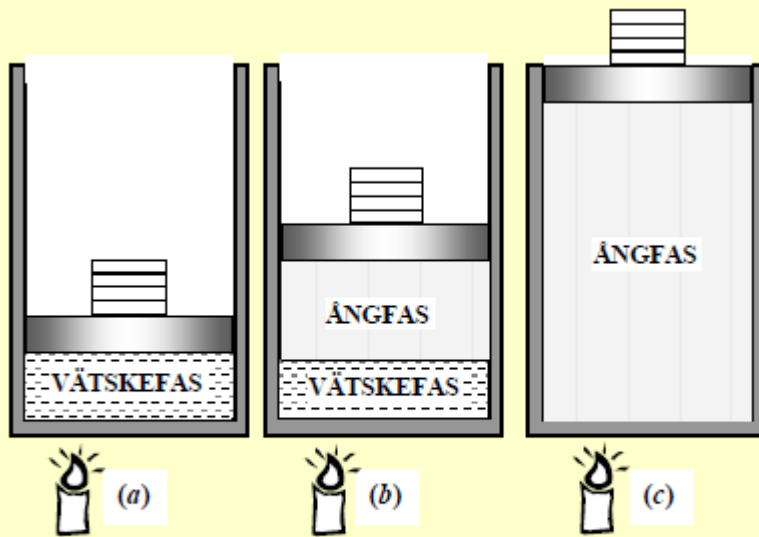
Verklig Ottocykel



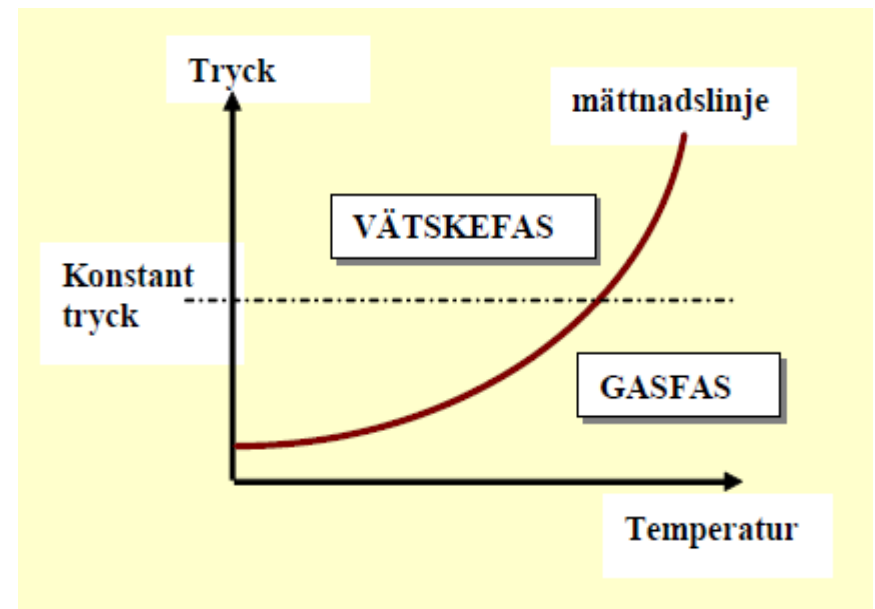
Dieselmotorn



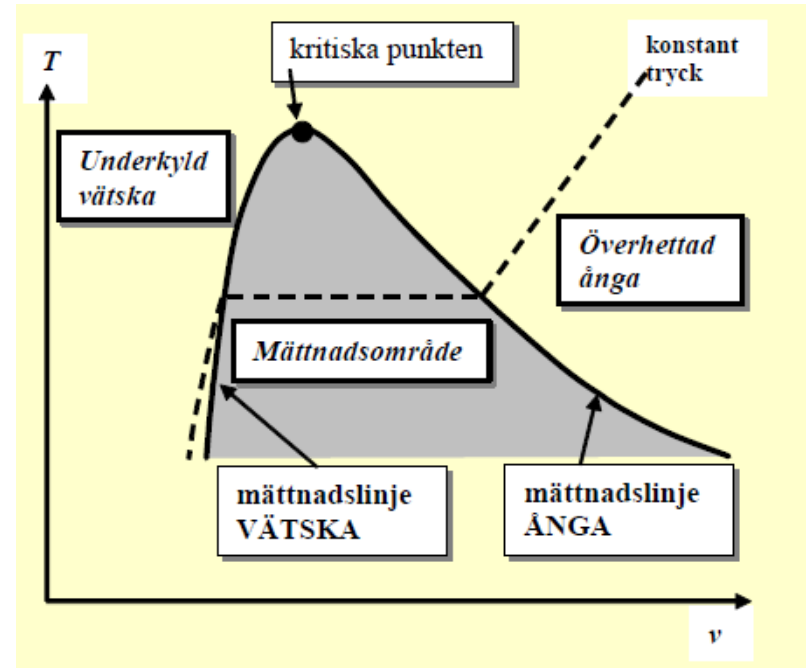
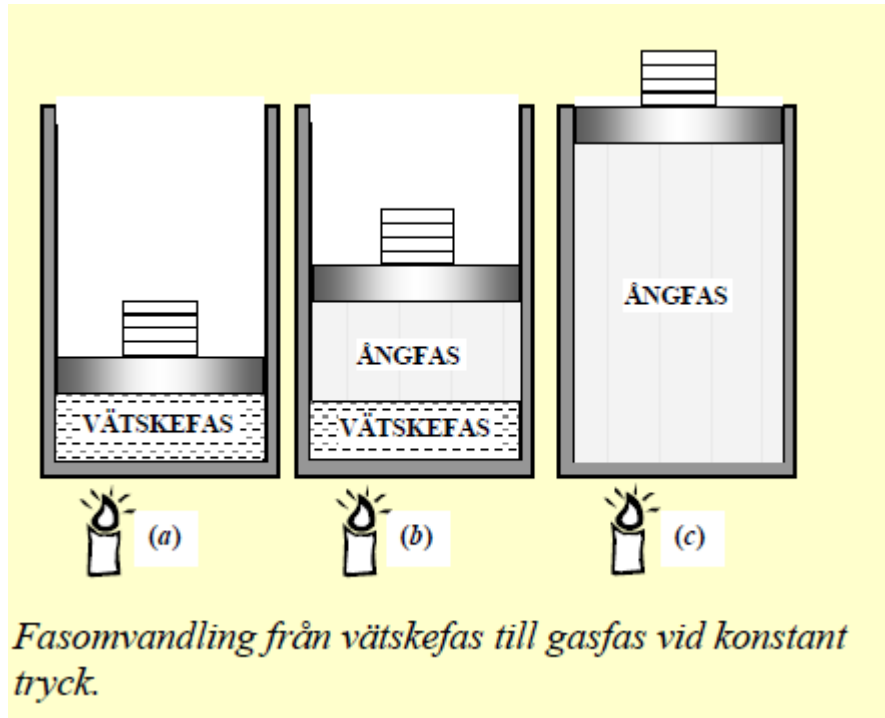
Fasdiagram för enkomponentsystem



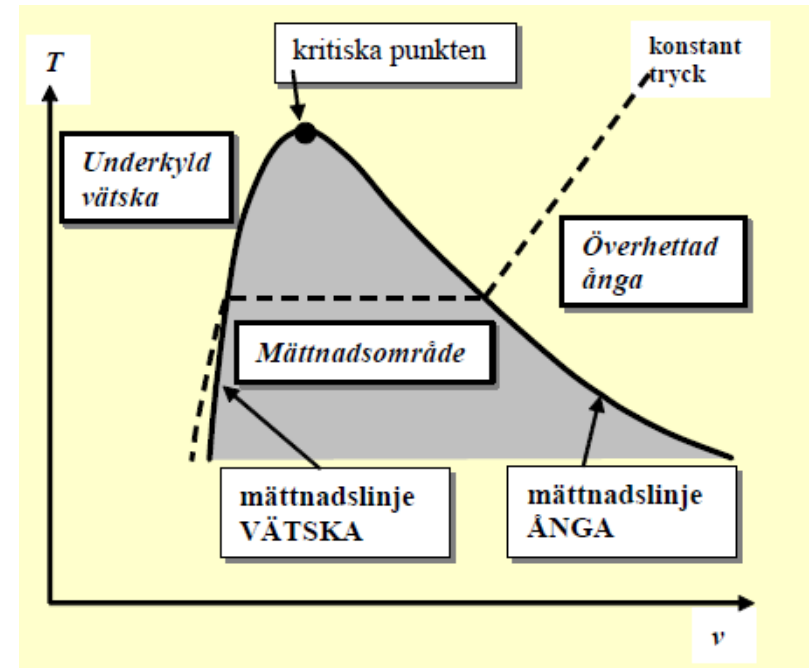
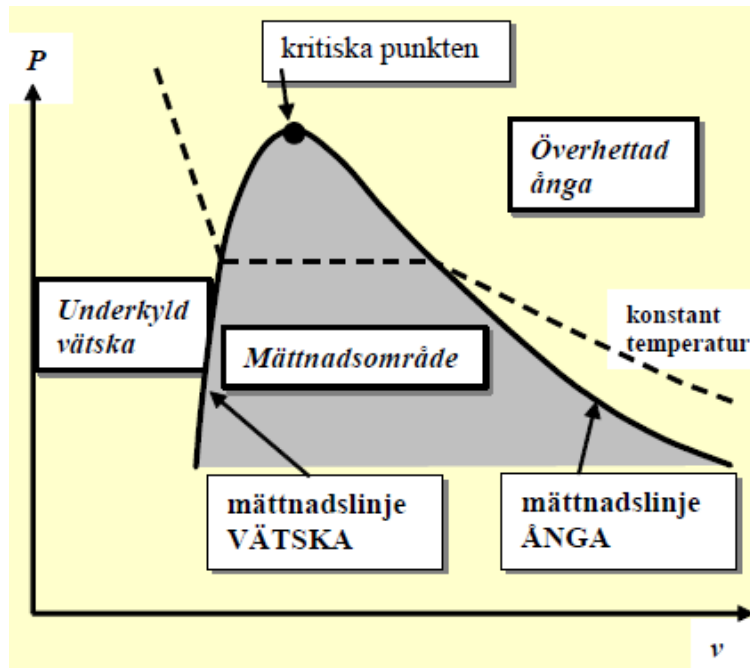
Fasomvandling från vätskefas till gasfas vid konstant tryck.



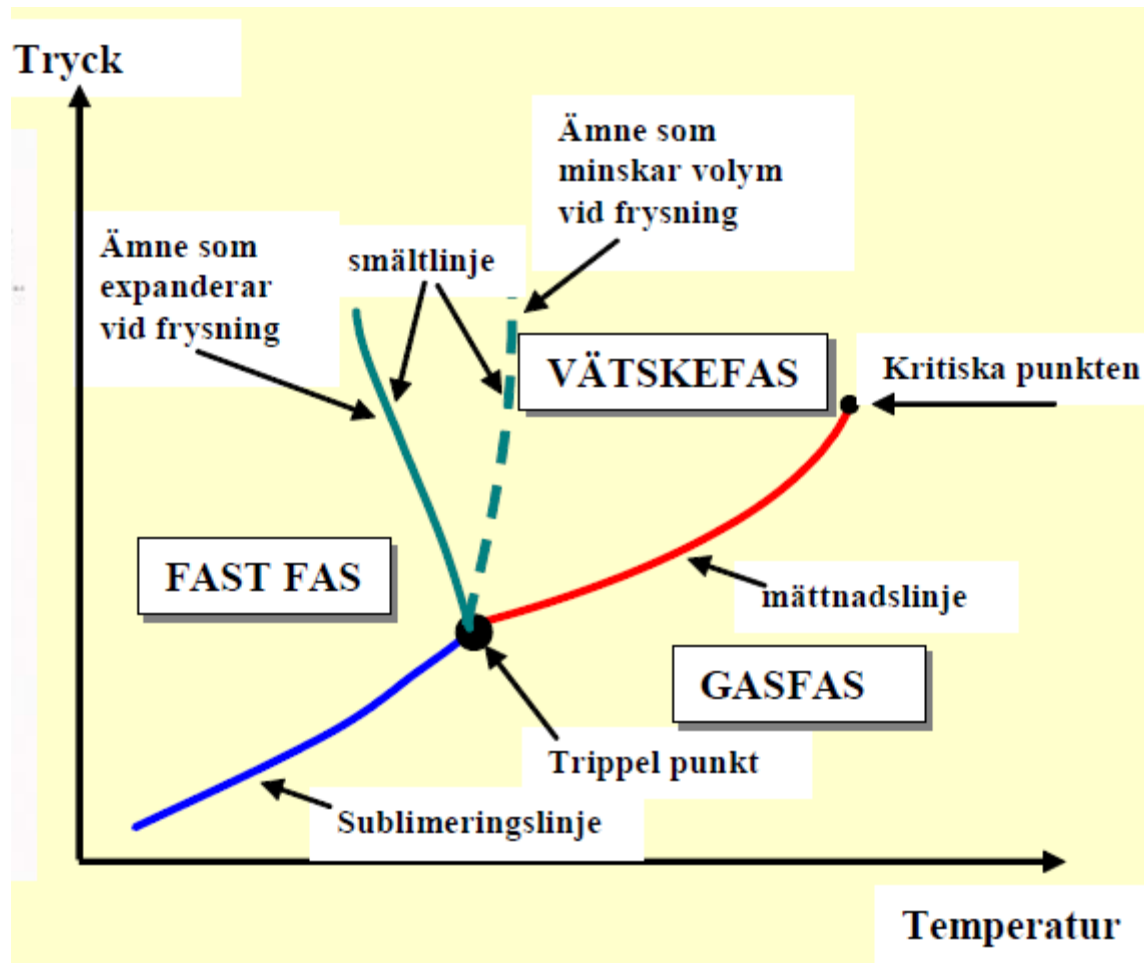
Fasdiagram för enkomponentsystem



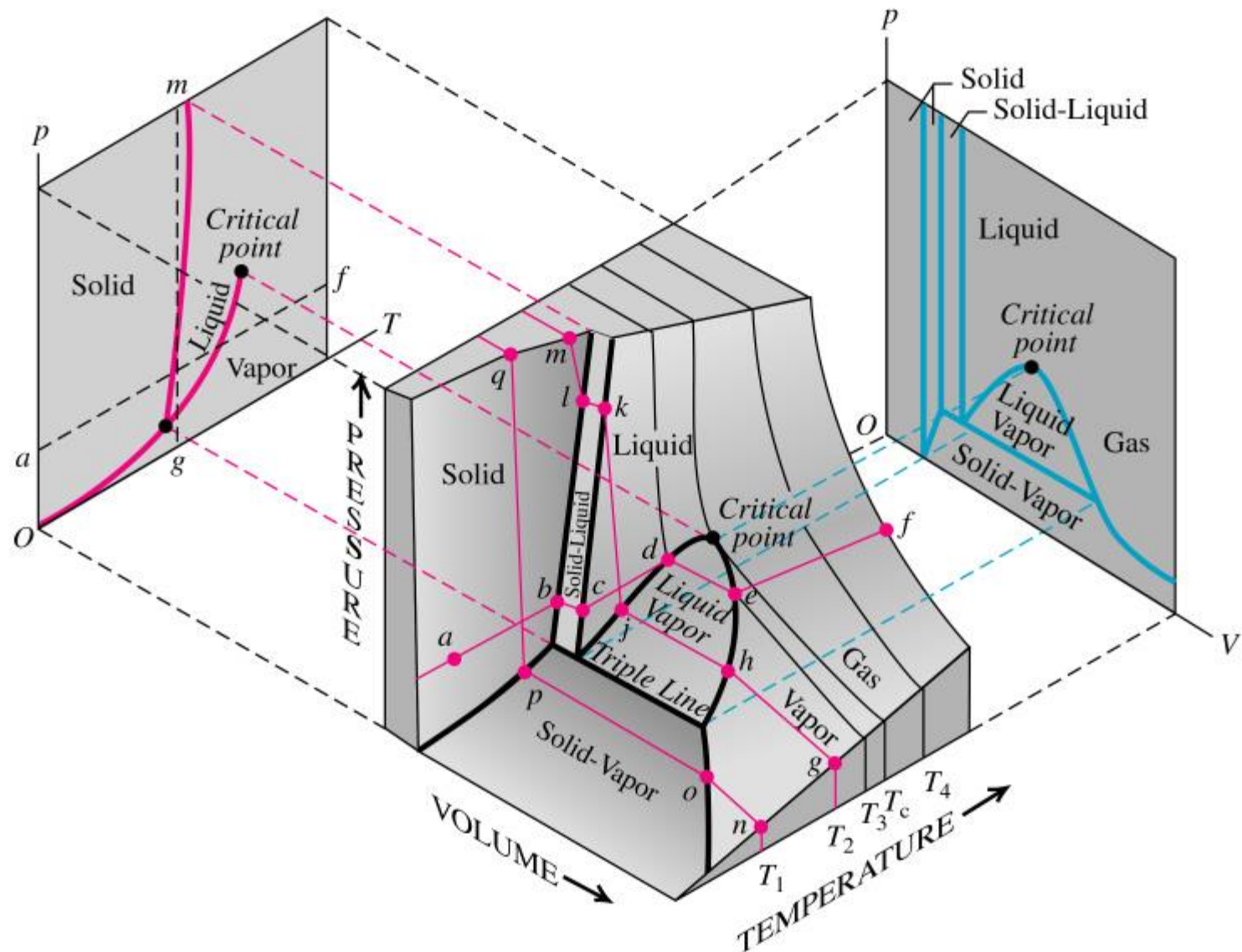
Fasdiagram för enkomponentsystem



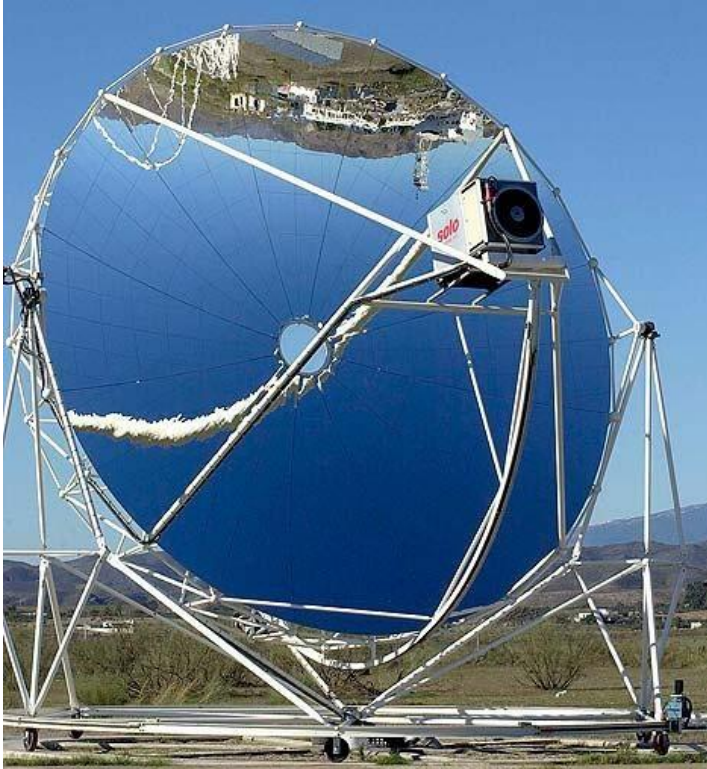
Fasdiagram för enkomponentsystem



Fasdiagramm för enkomponentsystem



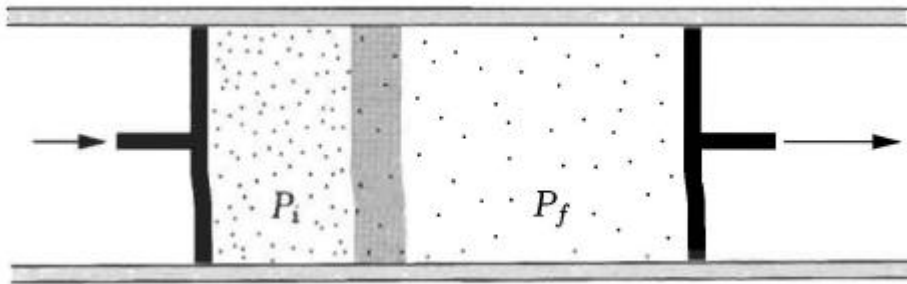
Hur omvandlas värme till
elenergi i en Stirlingmotor ?



Hur fungerar
kompressorkylskåpet ?

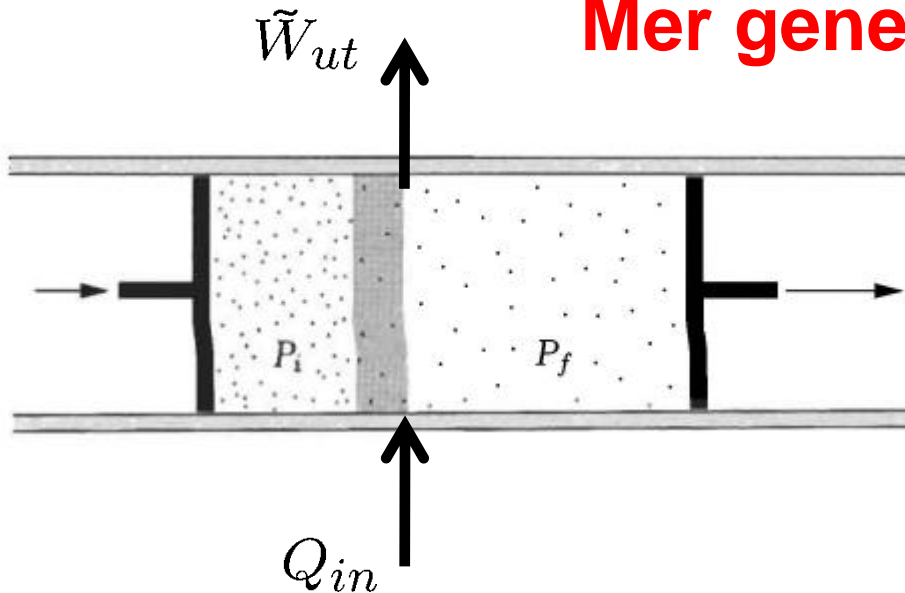


Joule-Thomson processen (strypning)



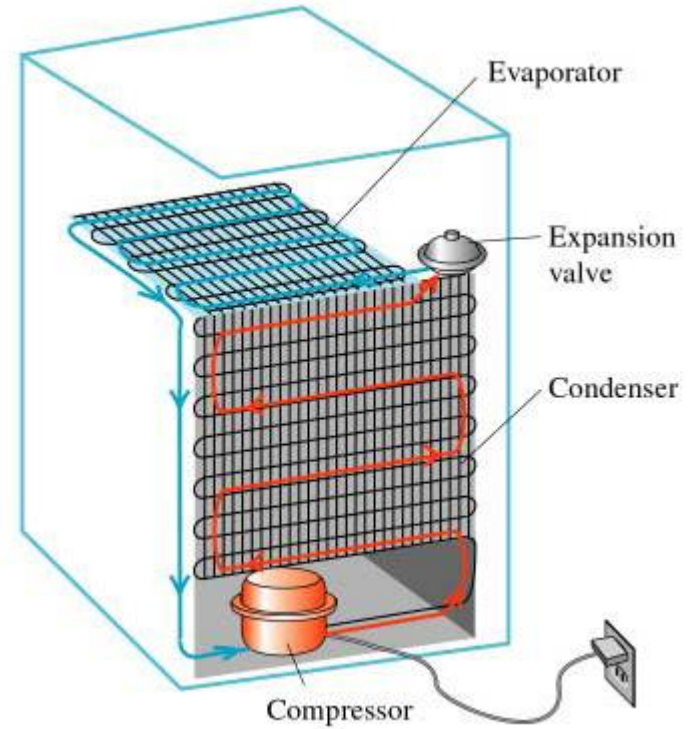
$$H_i = H_f$$

Mer generellt

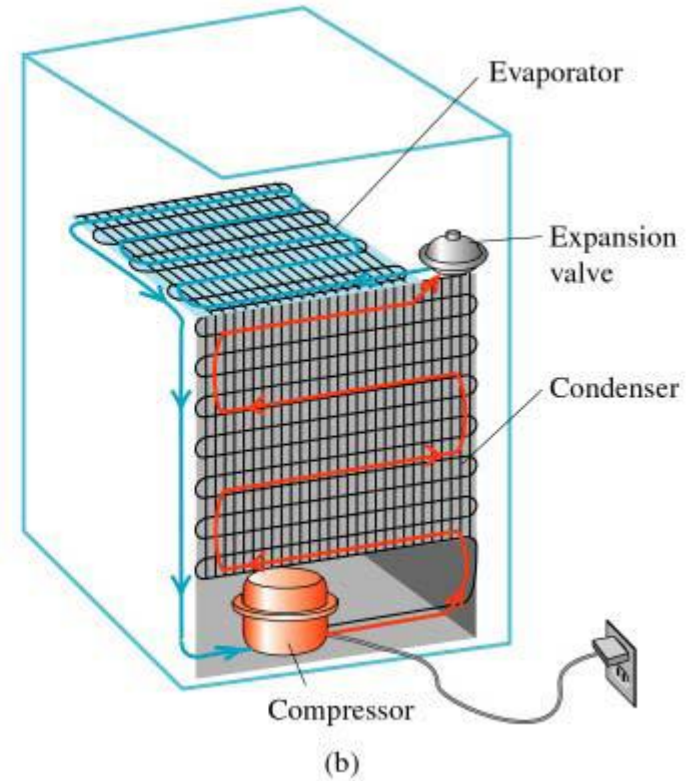
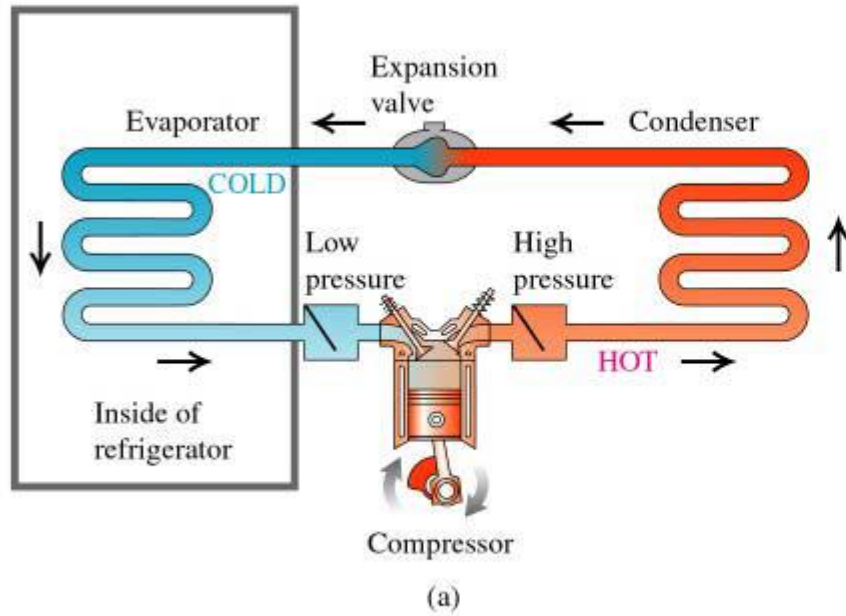


$$H_i + Q_{in} = H_f + \tilde{W}_{ut}$$

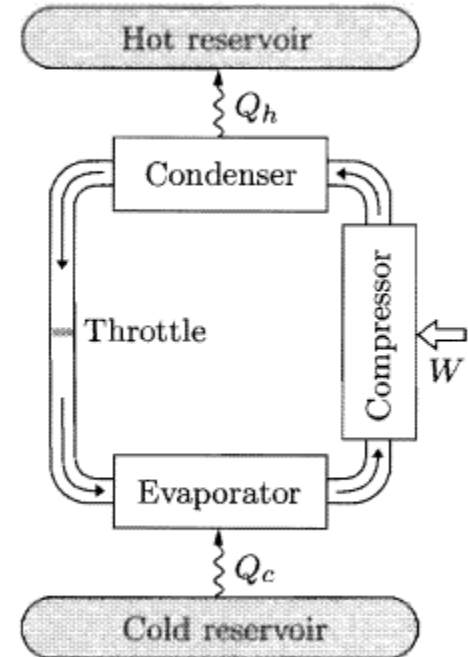
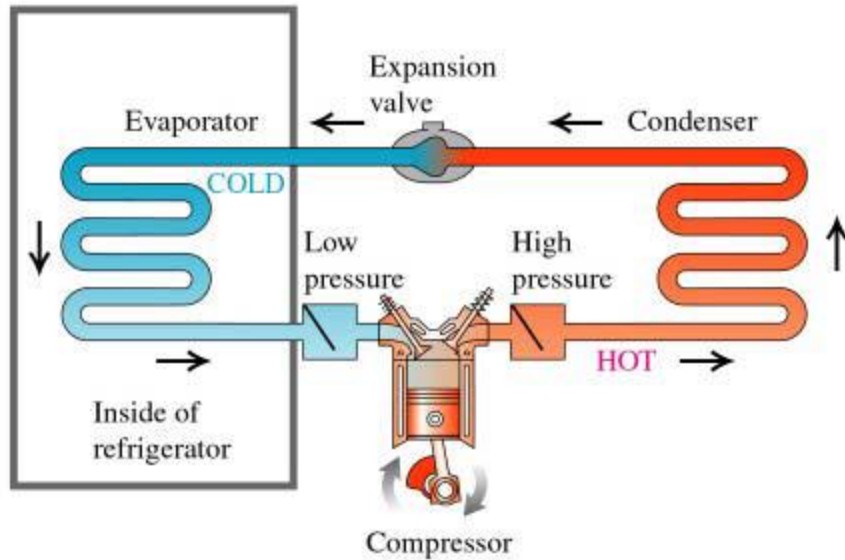
Kompressorkylskåp



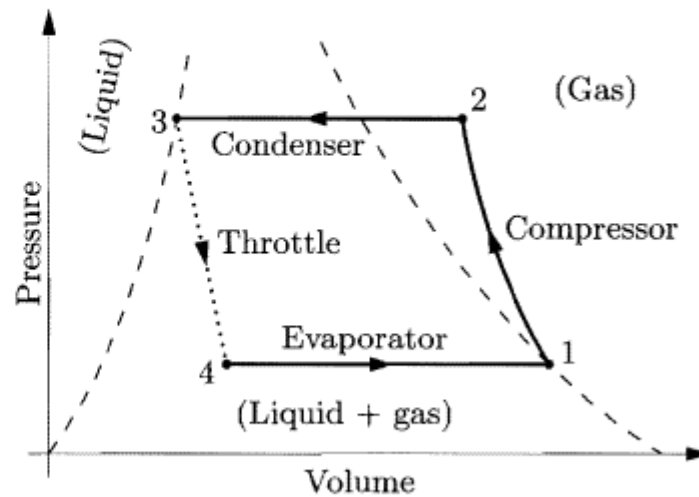
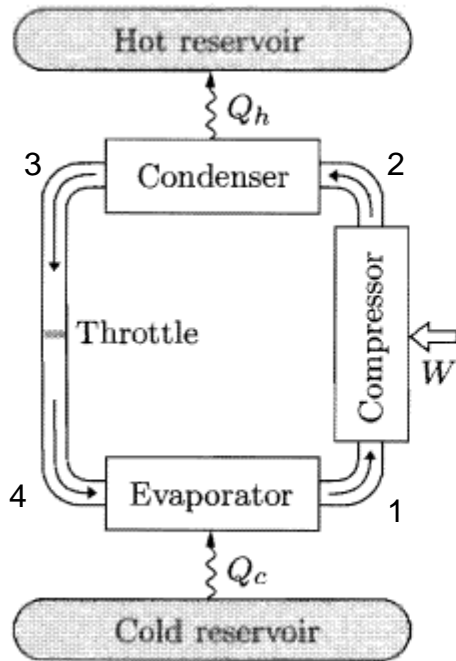
Kompressorkylskåp



Kompressorkylskåp



Kompressorkylskåp



Tabellerade värden

P (bar)	T (°C)	H_{liquid} (kJ)	H_{gas} (kJ)	S_{liquid} (kJ/K)	S_{gas} (kJ/K)
1.0	-26.4	16	231	0.068	0.940
1.4	-18.8	26	236	0.106	0.932
2.0	-10.1	37	241	0.148	0.925
4.0	8.9	62	252	0.240	0.915
6.0	21.6	79	259	0.300	0.910
8.0	31.3	93	264	0.346	0.907
10.0	39.4	105	268	0.384	0.904
12.0	46.3	116	271	0.416	0.902

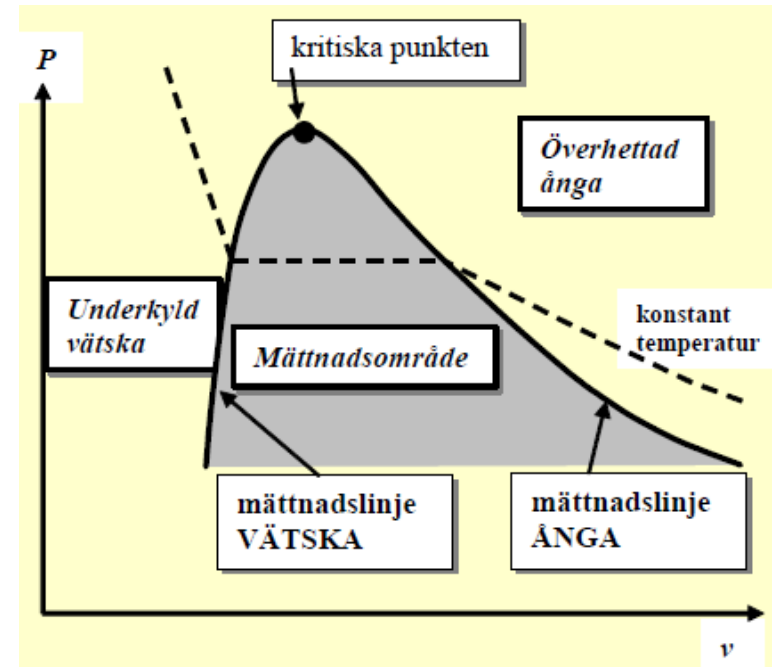
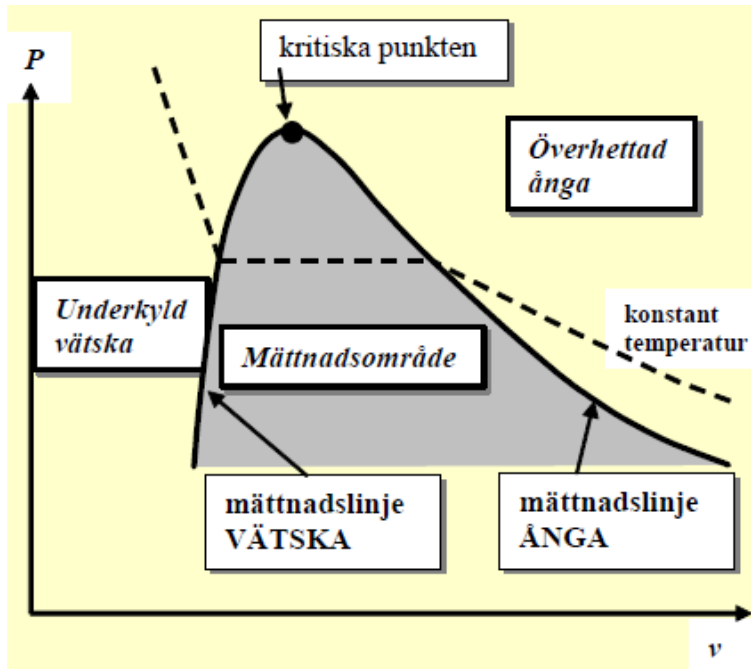


Table 4.3. Properties of the refrigerant HFC-134a under saturated conditions (at its boiling point for each pressure). All values are for 1 kg of fluid, and are measured relative to an arbitrarily chosen reference state, the saturated liquid at -40°C . Excerpted from Moran and Shapiro (1995).

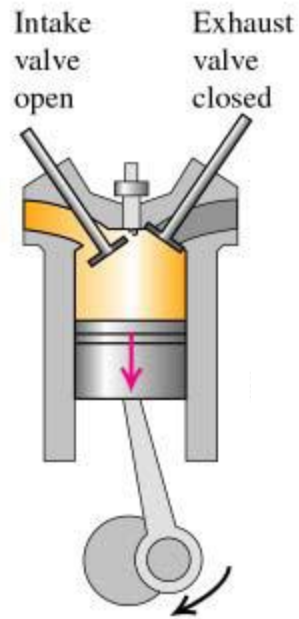
Tabellerade värden



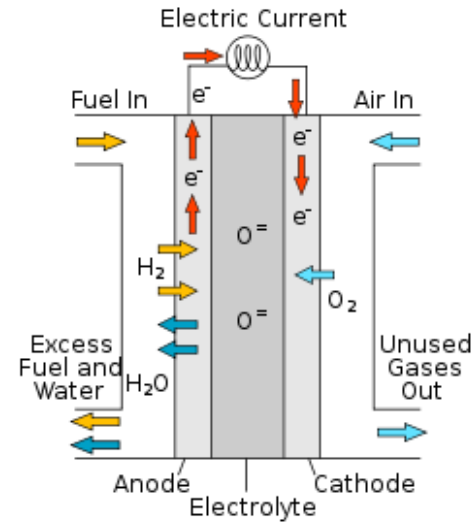
P (bar)		Temperature (°C)		
		40	50	60
8.0	H (kJ)	274	284	295
	S (kJ/K)	0.937	0.971	1.003
10.0	H (kJ)	269	280	291
	S (kJ/K)	0.907	0.943	0.977
12.0	H (kJ)		276	287
	S (kJ/K)		0.916	0.953

Table 4.4. Properties of superheated (gaseous) refrigerant HFC-134a. All values are for 1 kg of fluid, and are measured relative to the same reference state as in Table 4.3. Excerpted from Moran and Shapiro (1995).

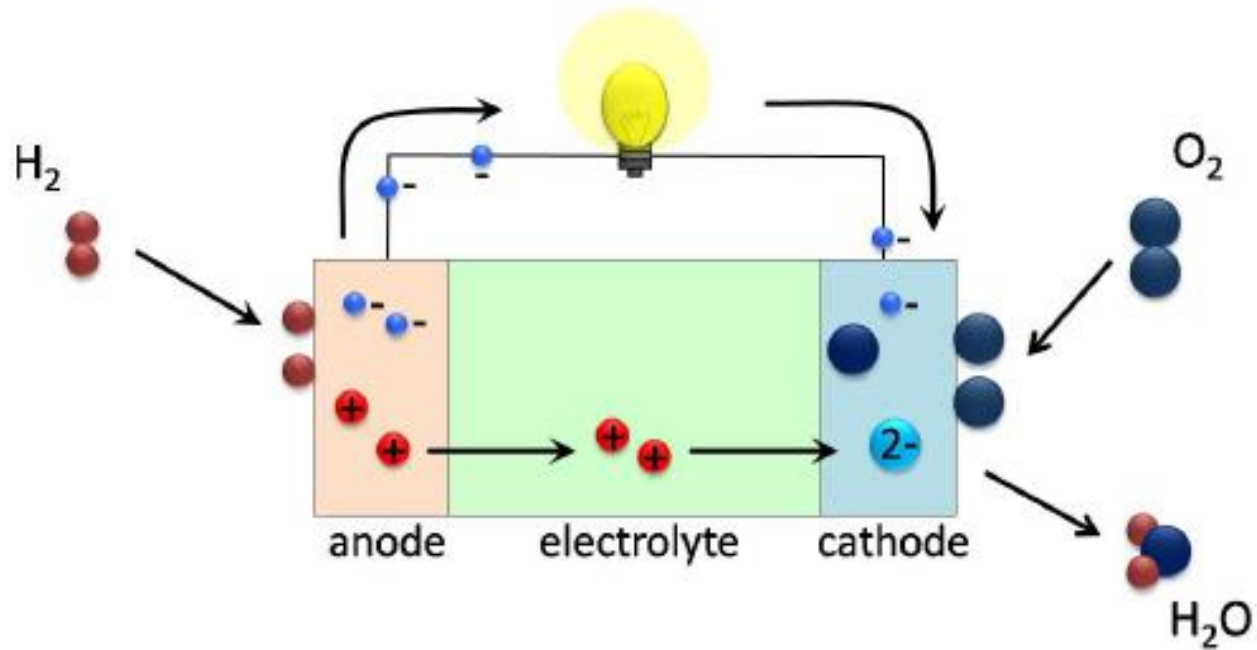
Ottomotorn



Hur fungerar en bränslecell ?



Bränslecell



Termodynamikens huvudsatser

Första huvudsatsen

$$\Delta U = Q + W$$

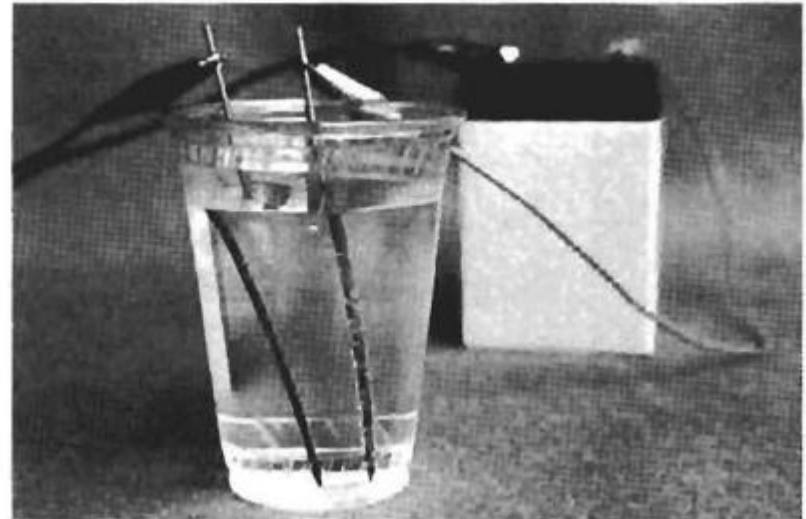
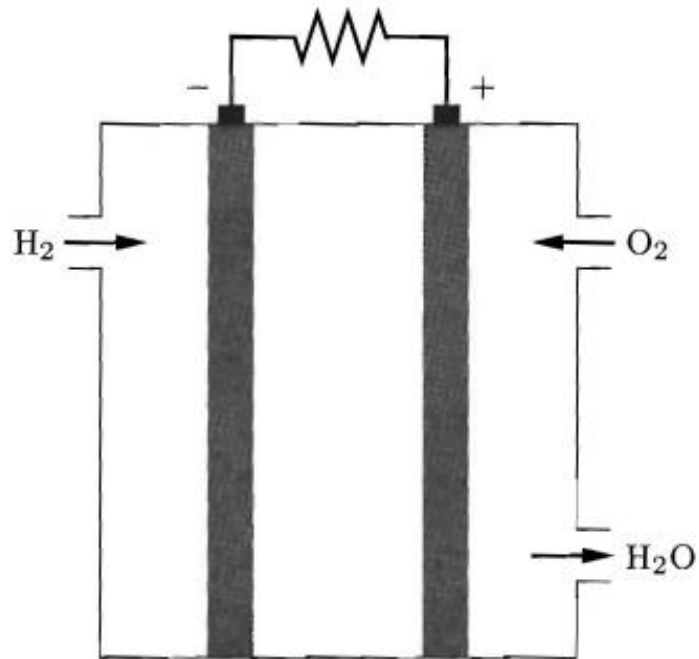
Isolerat system: $\Delta U = 0$

Andra huvudsatsen

$$\Delta S \geq \frac{Q}{T}$$

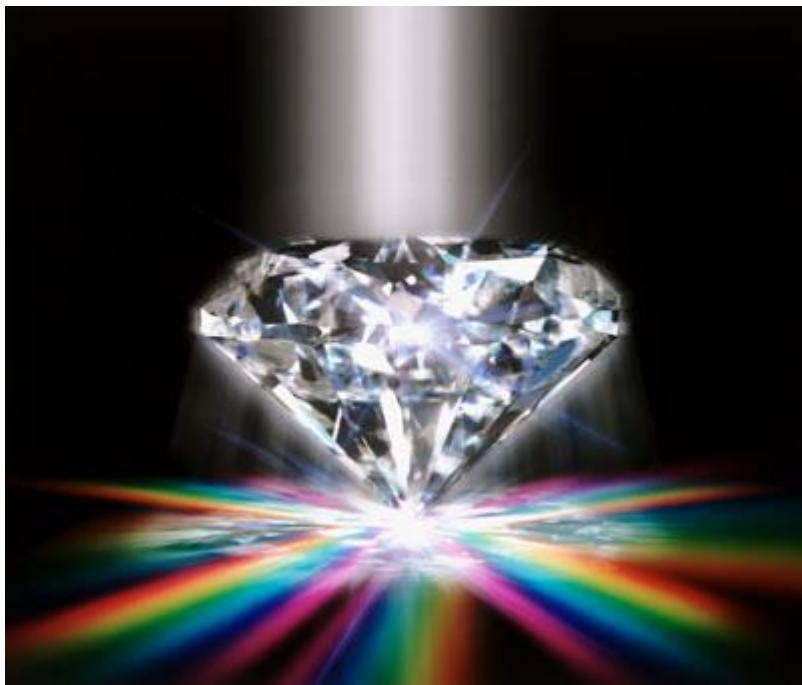
Isolerat system: $\Delta S \geq 0$

Bränslecell \longleftrightarrow Elektrolys



Substance (form)	$\Delta_f H$ (kJ)	$\Delta_f G$ (kJ)	S (J/K)	C_P (J/K)	V (cm ³)
H ₂ (g)	0	0	130.68	28.82	
H (g)	217.97	203.25	114.71	20.78	
H ⁺ (aq)	0	0	0	0	
H ₂ O (l)	-285.83	-237.13	69.91	75.29	18.068
H ₂ O (g)	-241.82	-228.57	188.83	33.58	
He (g)	0	0	126.15	20.79	
Hg (l)	0	0	76.02	27.98	14.81
N ₂ (g)	0	0	191.61	29.12	
NH ₃ (g)	-46.11	-16.45	192.45	35.06	
Na ⁺ (aq)	-240.12	-261.91	59.0	46.4	-1.2
NaCl (s)	-411.15	-384.14	72.13	50.50	27.01
NaAlSi ₃ O ₈ (albite)	-3935.1	-3711.5	207.40	205.10	100.07
NaAlSi ₂ O ₆ (jadeite)	-3030.9	-2852.1	133.5	160.0	60.40
Ne (g)	0	0	146.33	20.79	
O ₂ (g)	0	0	205.14	29.38	

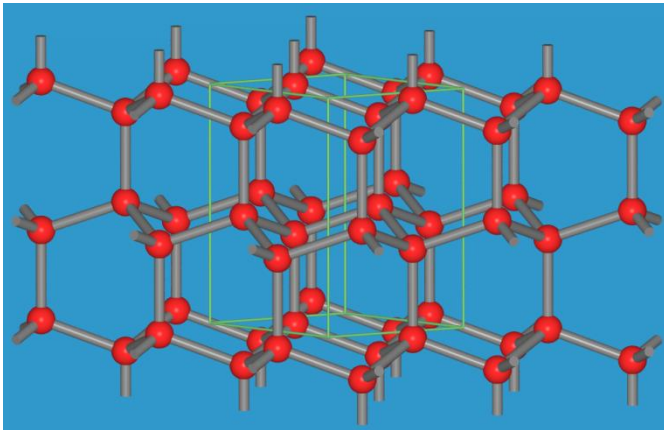
Hur påverkas diamants stabilitet
av tryckförändringar ?



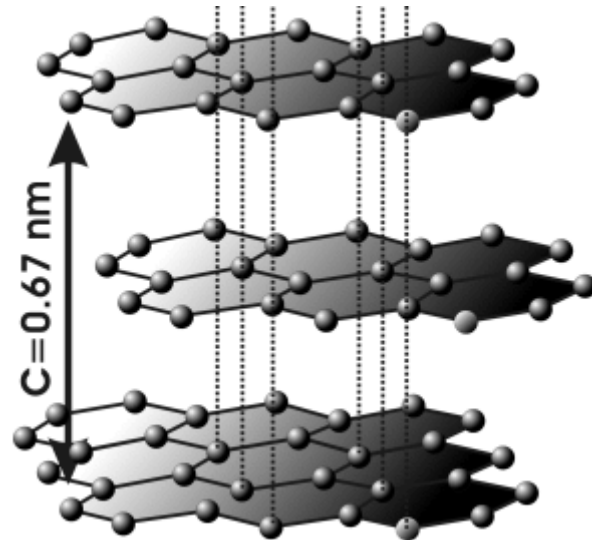
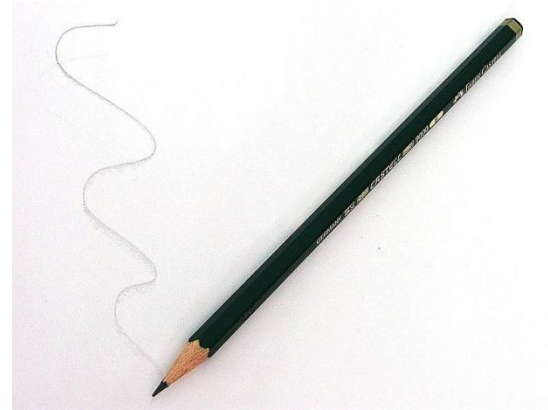
Smälter isen under skridskon ?



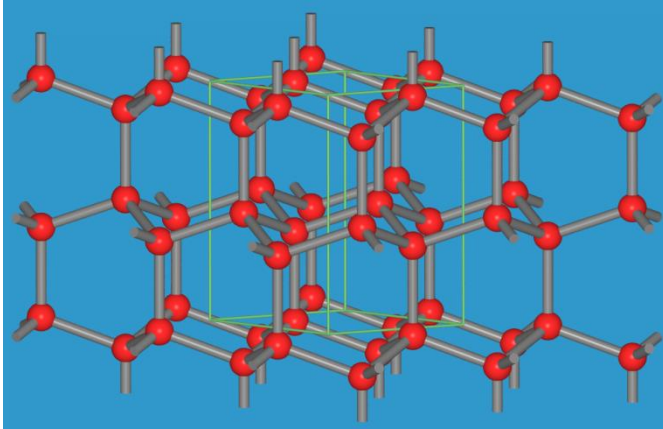
Diamant



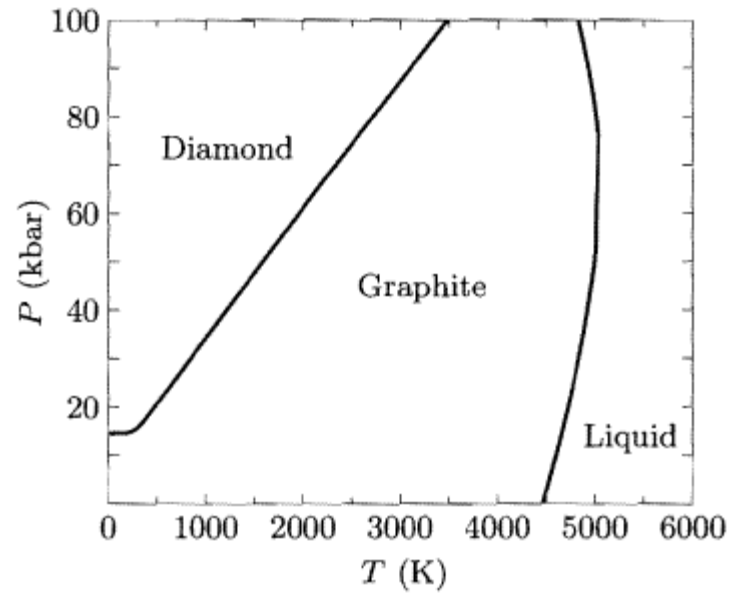
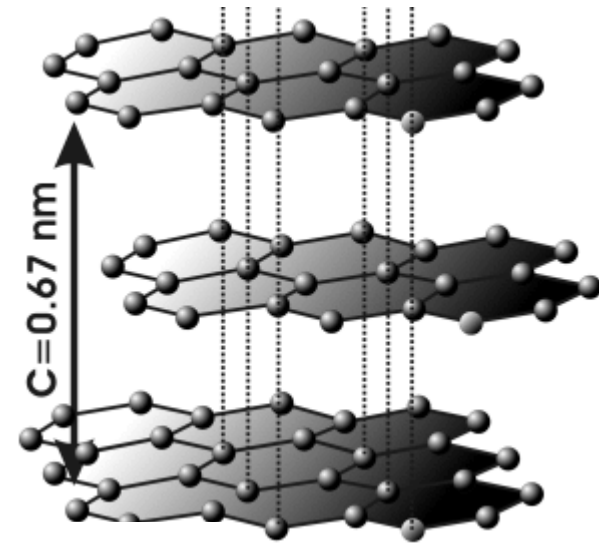
Grafit



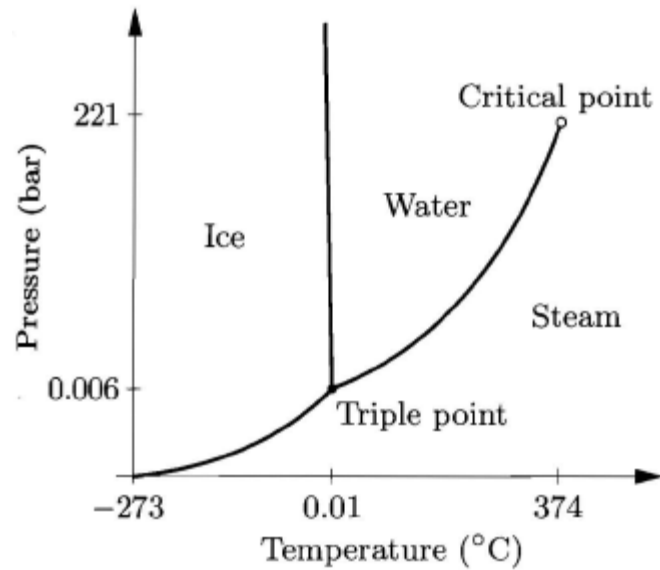
Diamant



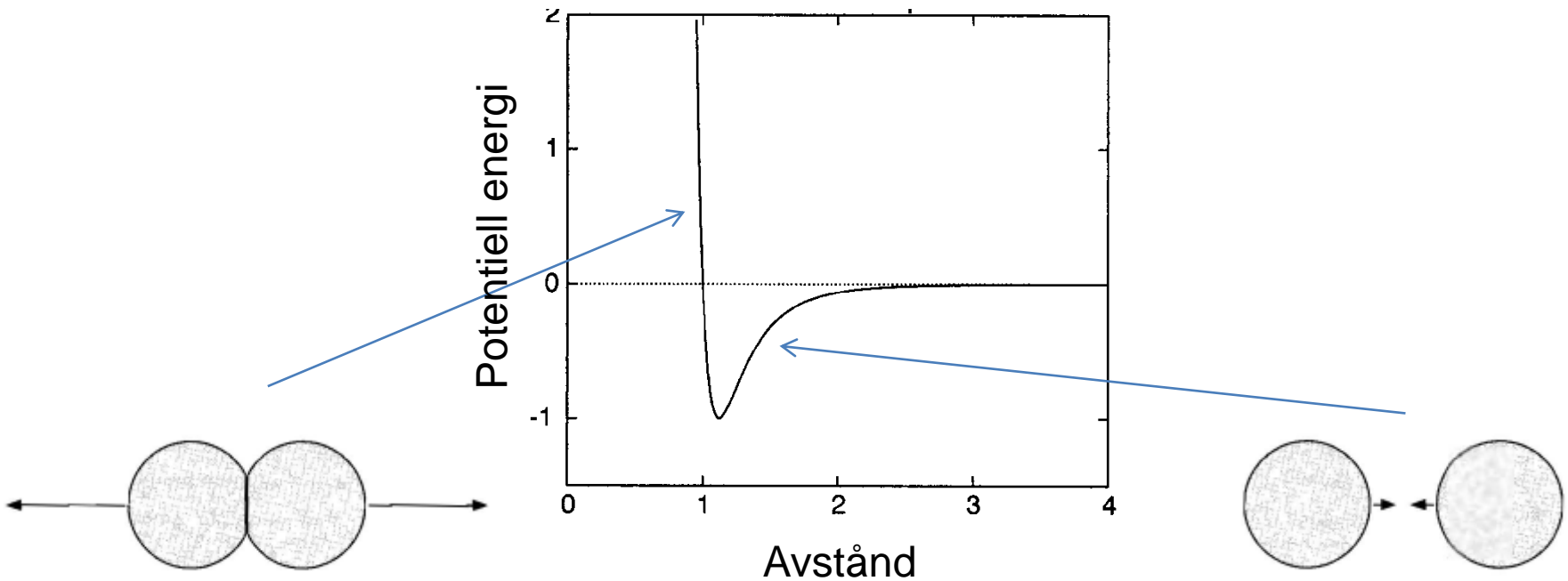
Grafit



Fasdiagramm för vatten

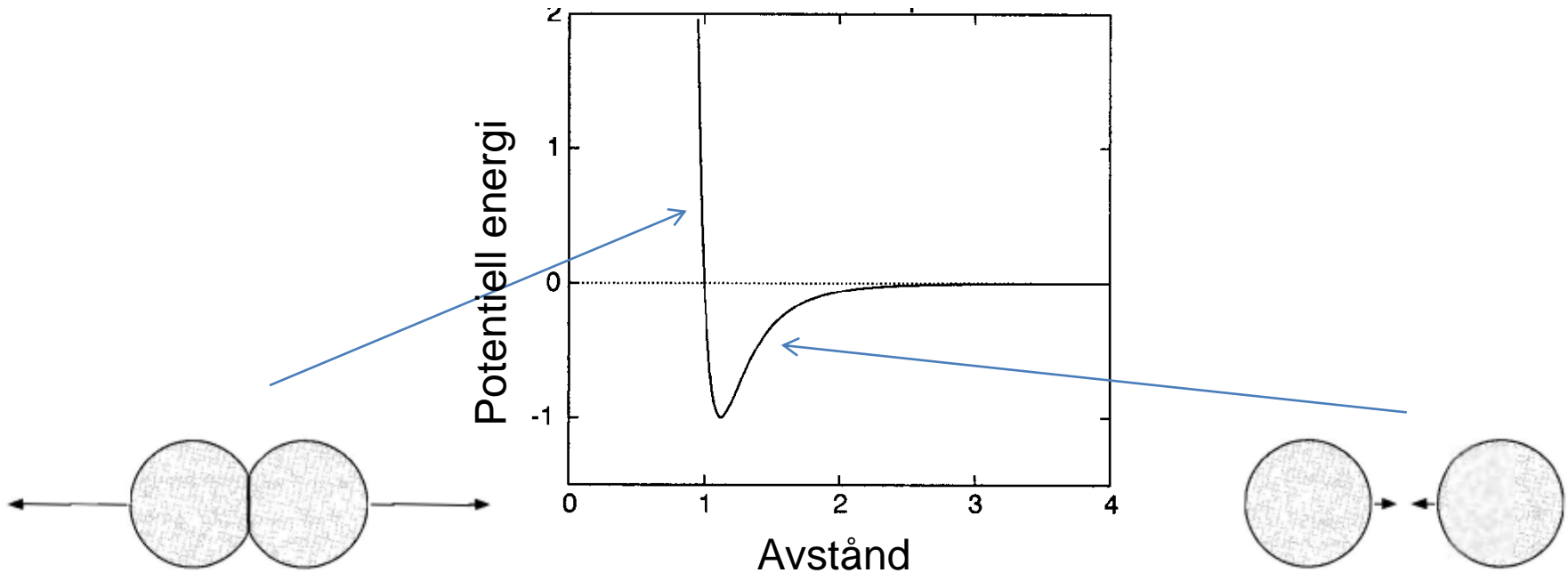


Växelverkan mellan molekyler



van der Waals tillståndsekvation

$$P = \frac{NkT}{V - Nb} - \frac{aN^2}{V^2}$$



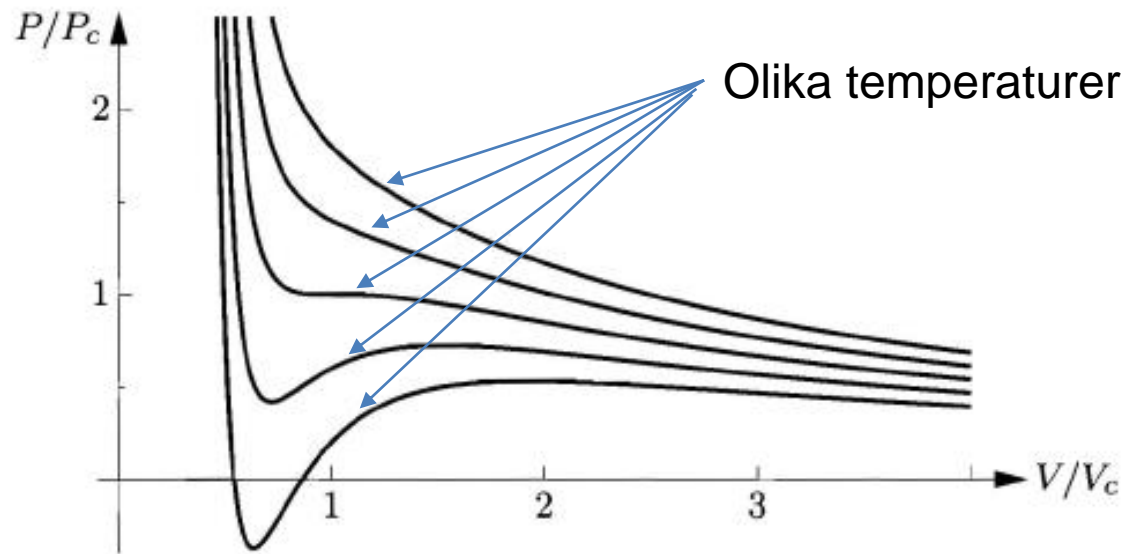
van der Waals tillståndsekvation

$$P = \frac{NkT}{V - Nb} - \frac{aN^2}{V^2}$$

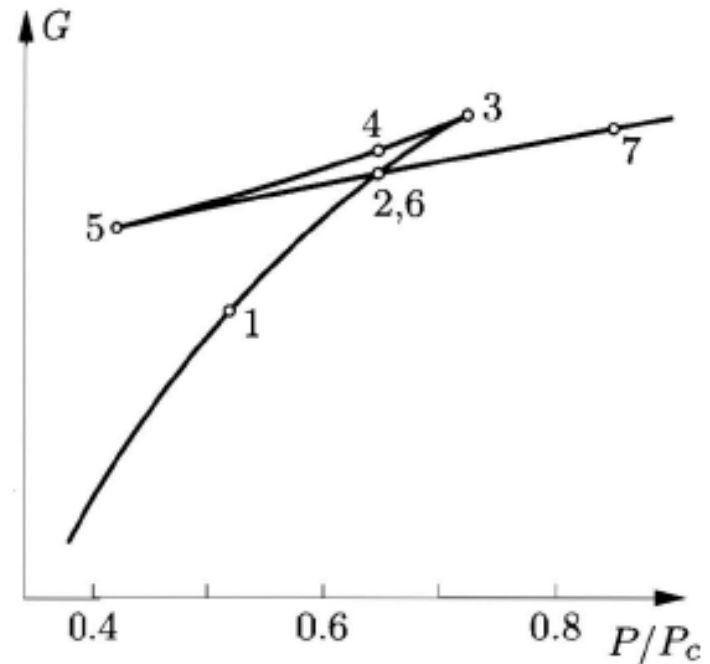
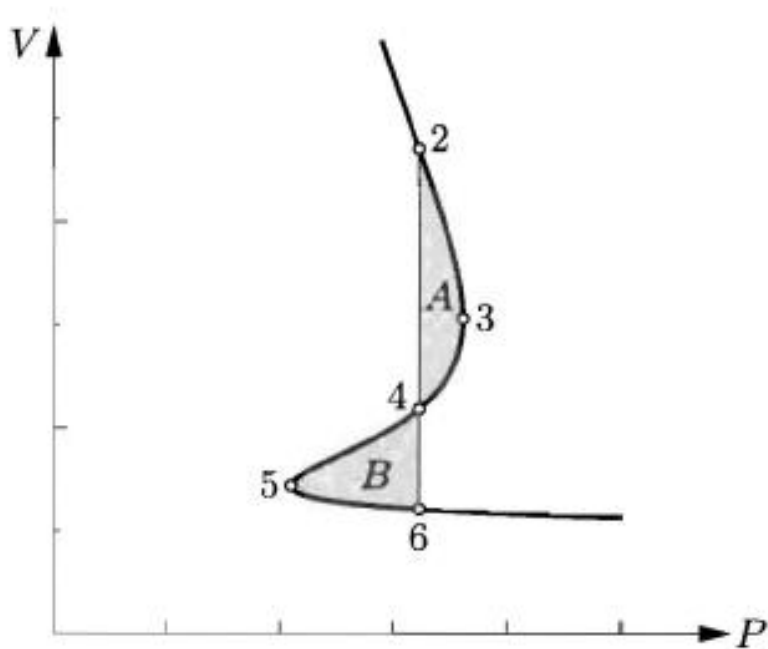
	a (eVÅ ³)	b (Å ³)	a/b (meV)
He	0.06	40	1.5
O ₂	2.4	53	45
N ₂	2.4	65	46
H ₂ O	9.5	51	188

van der Waals tillståndsekvation

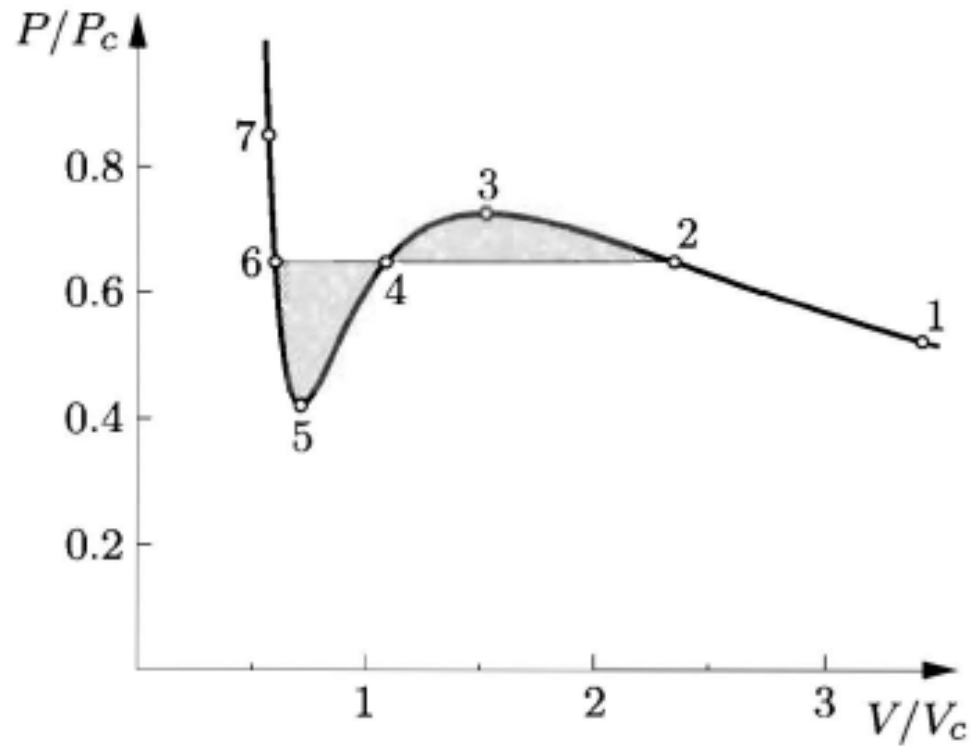
$$P = \frac{NkT}{V - Nb} - \frac{aN^2}{V^2}$$



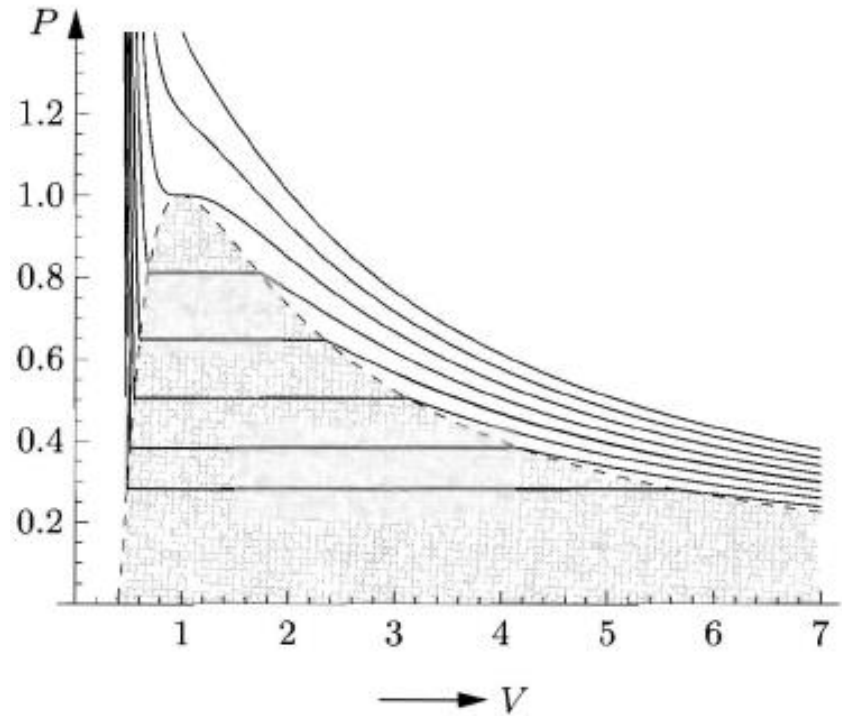
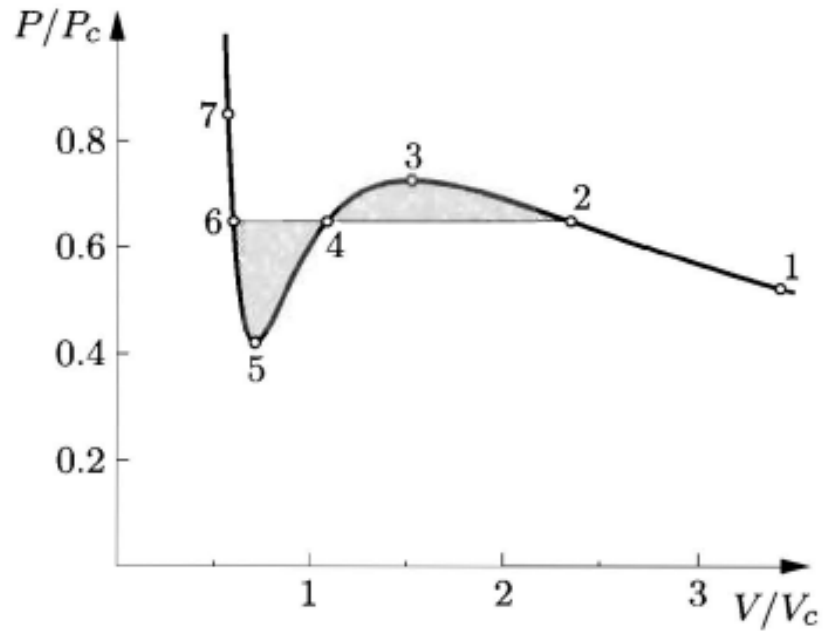
van der Waals tillståndsekvation



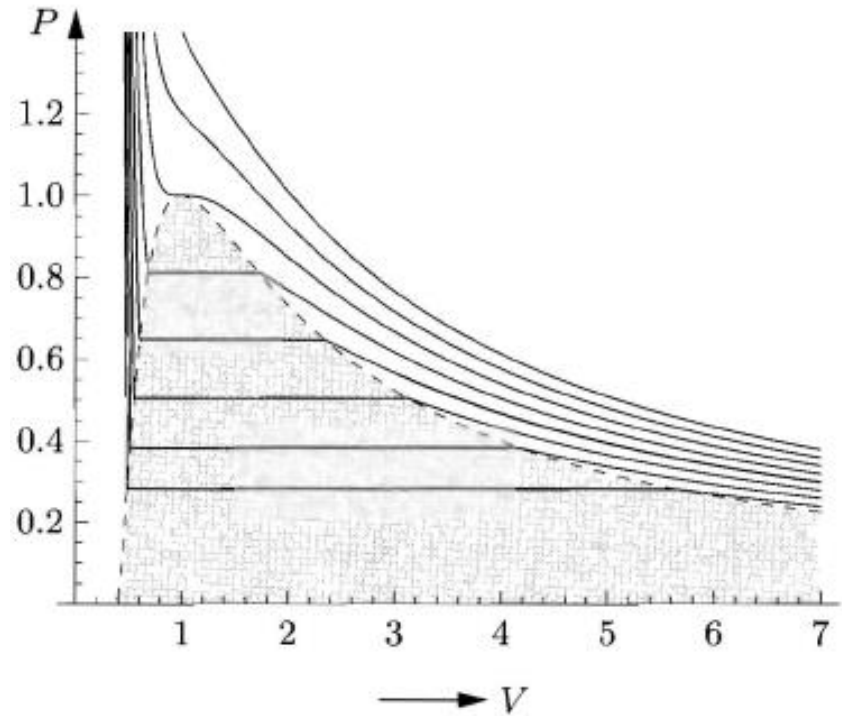
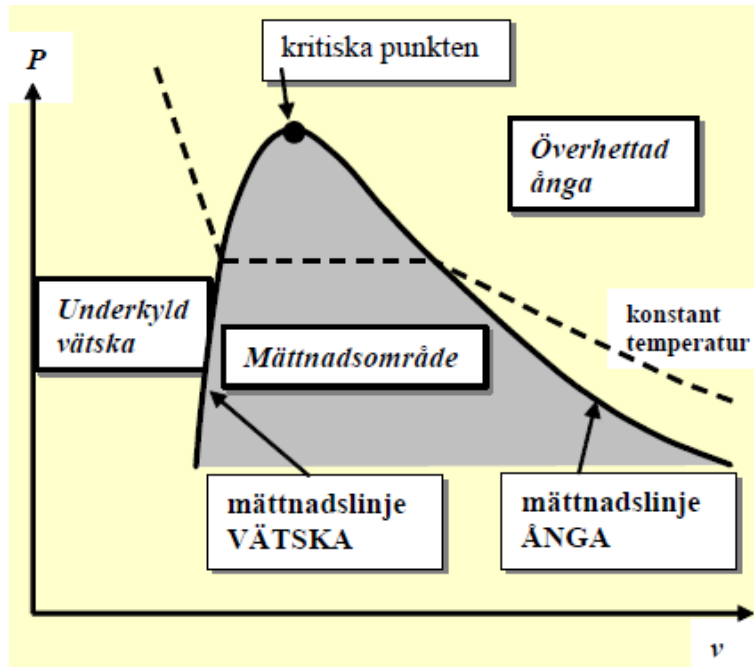
van der Waals tillståndsekvation



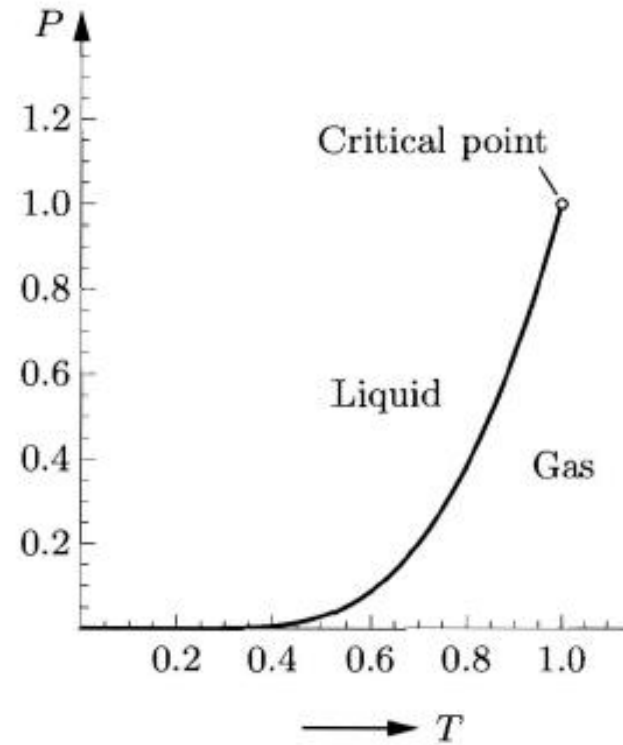
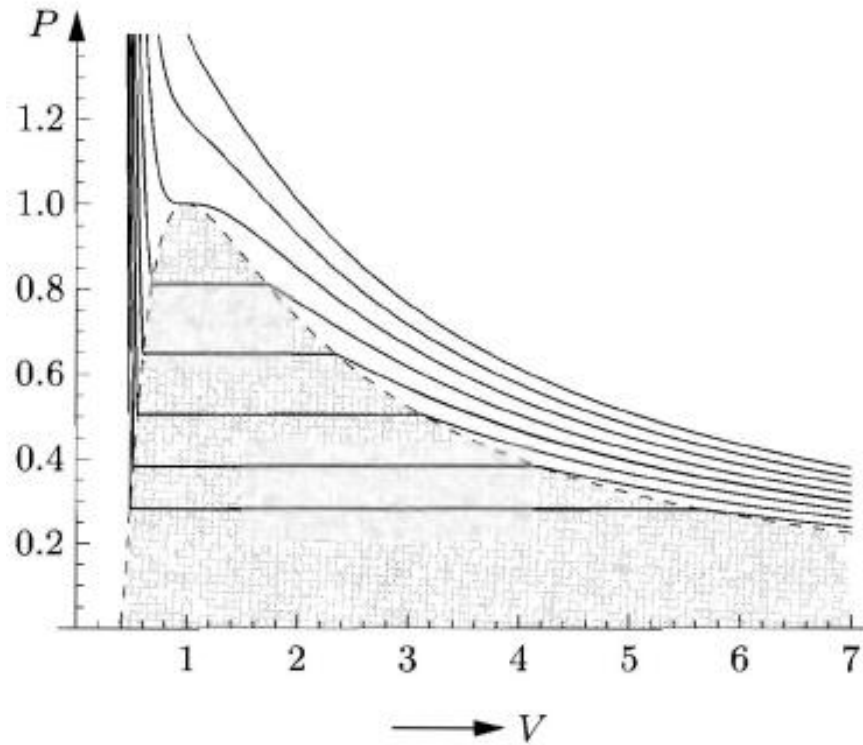
Maxwell konstruktioner



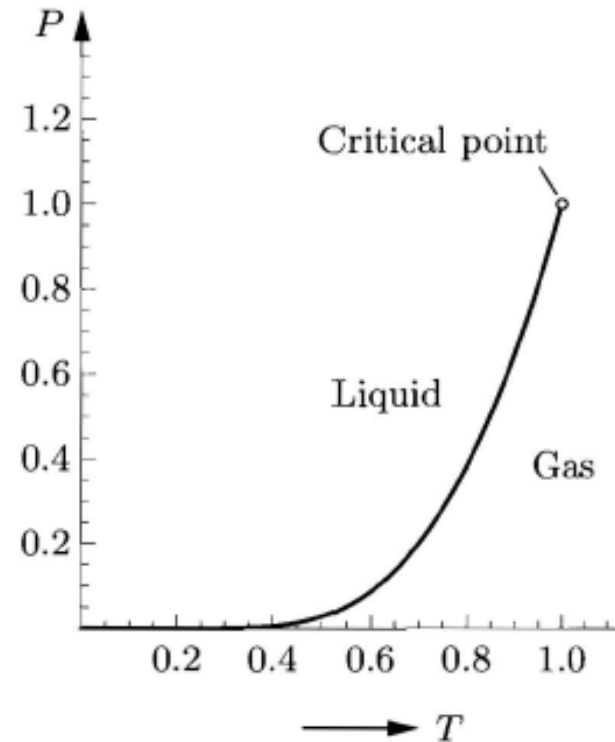
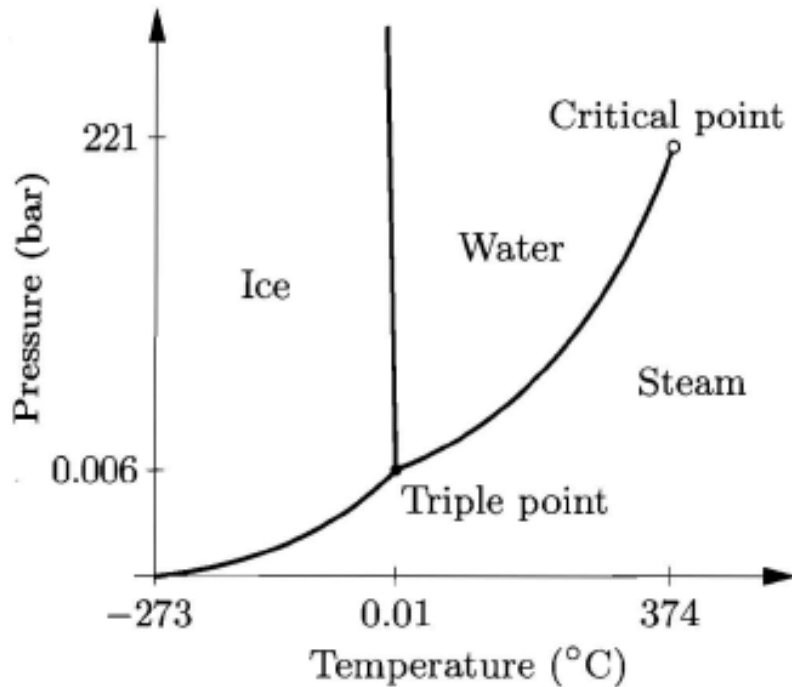
Maxwell konstruktionen



van der Waals tillståndsdigram



van der Waals tillståndsdigram



När fryser kylarvätskan ?



Vatten:

$$T_m = 0^{\circ}\text{C}$$

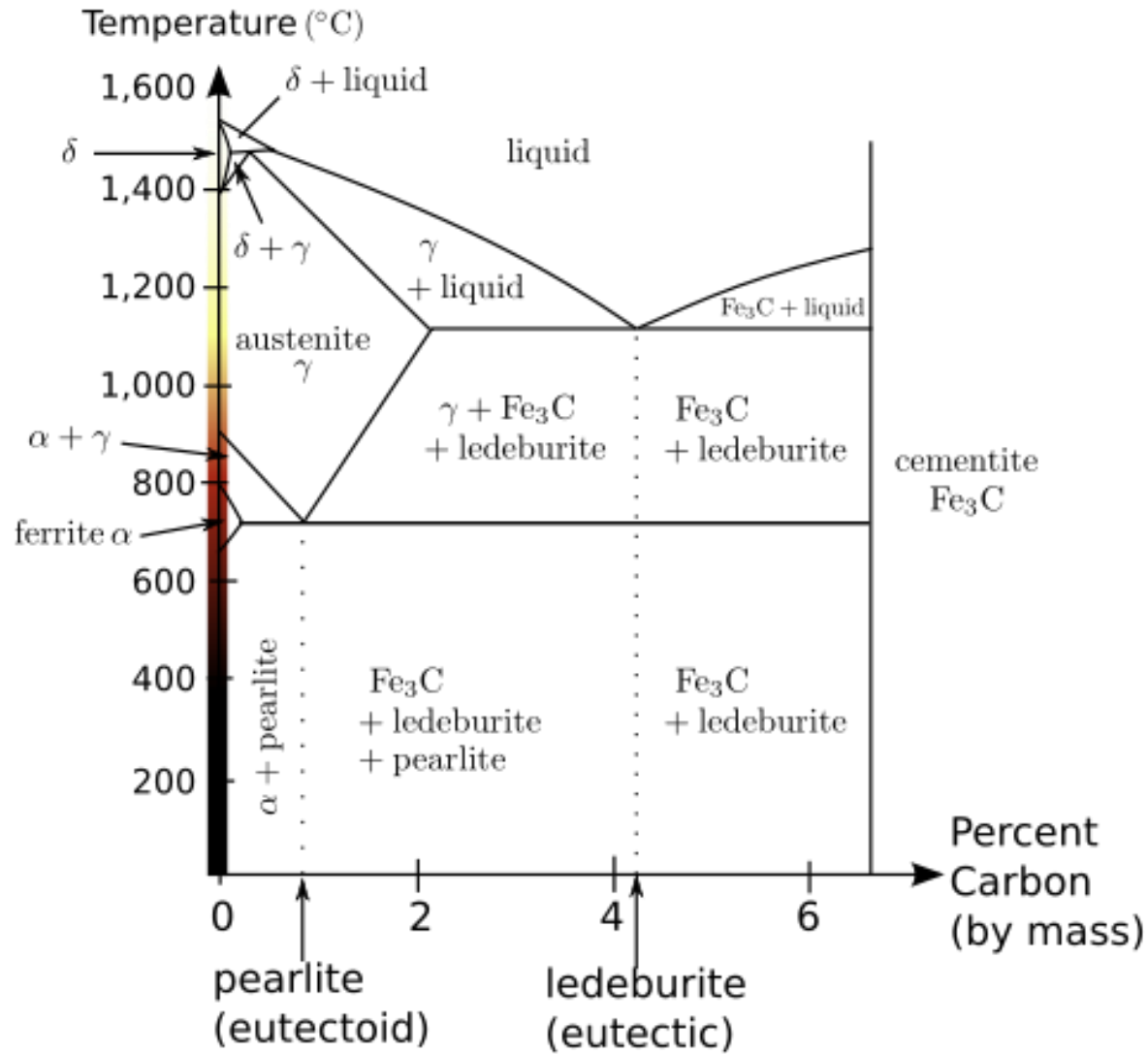
Glykol:

$$T_m = -13^{\circ}\text{C}$$

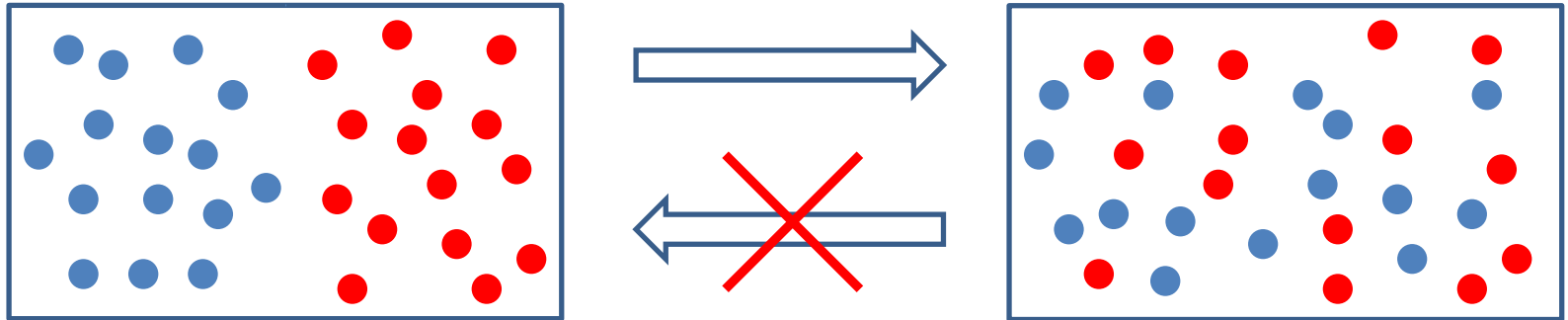
Kylarvätska (vatten och glykol):

$$\min[T_m] = -49^{\circ}\text{C}$$

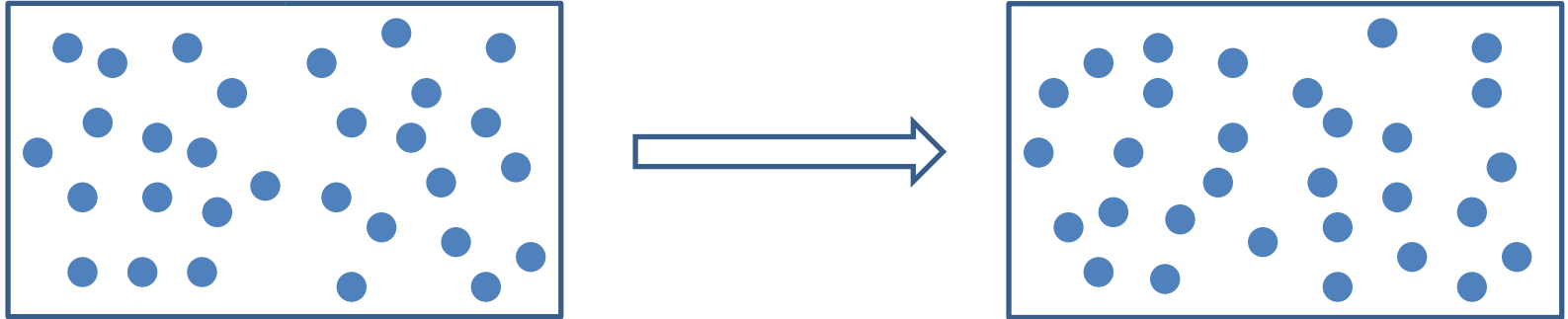
Stål



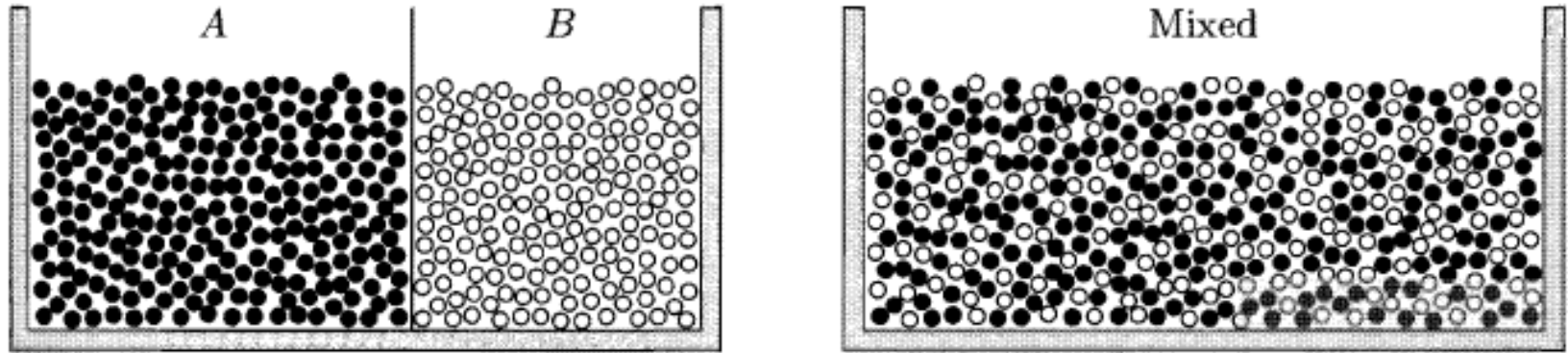
Irreversibel process



Irreversibel process ?

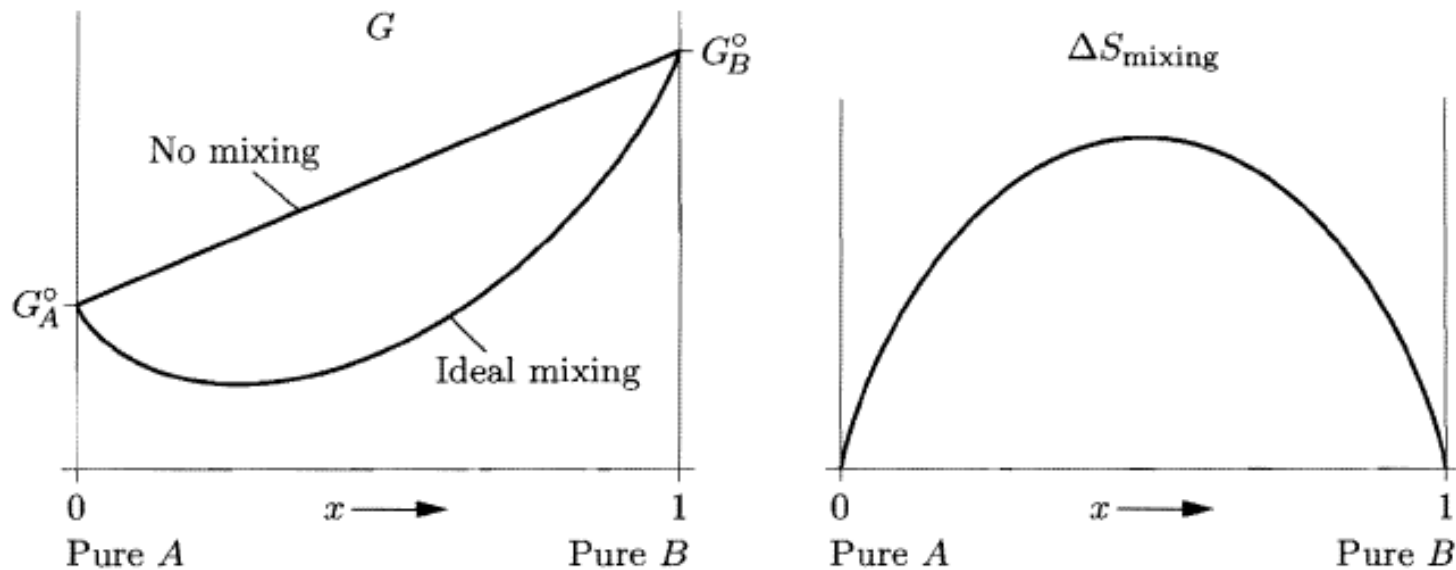


Blandningsentropi

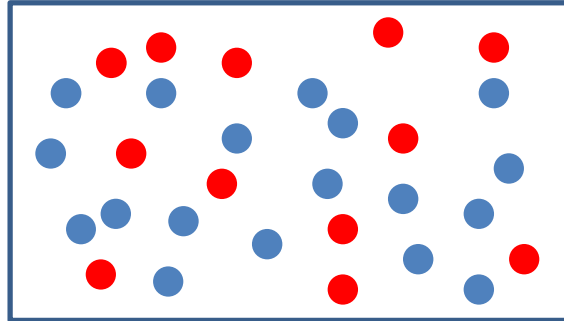


Ideal blandning

$$G = (1-x)G_A^o + xG_B^o + RT[x \ln x + (1-x) \ln (1-x)]$$



Luft

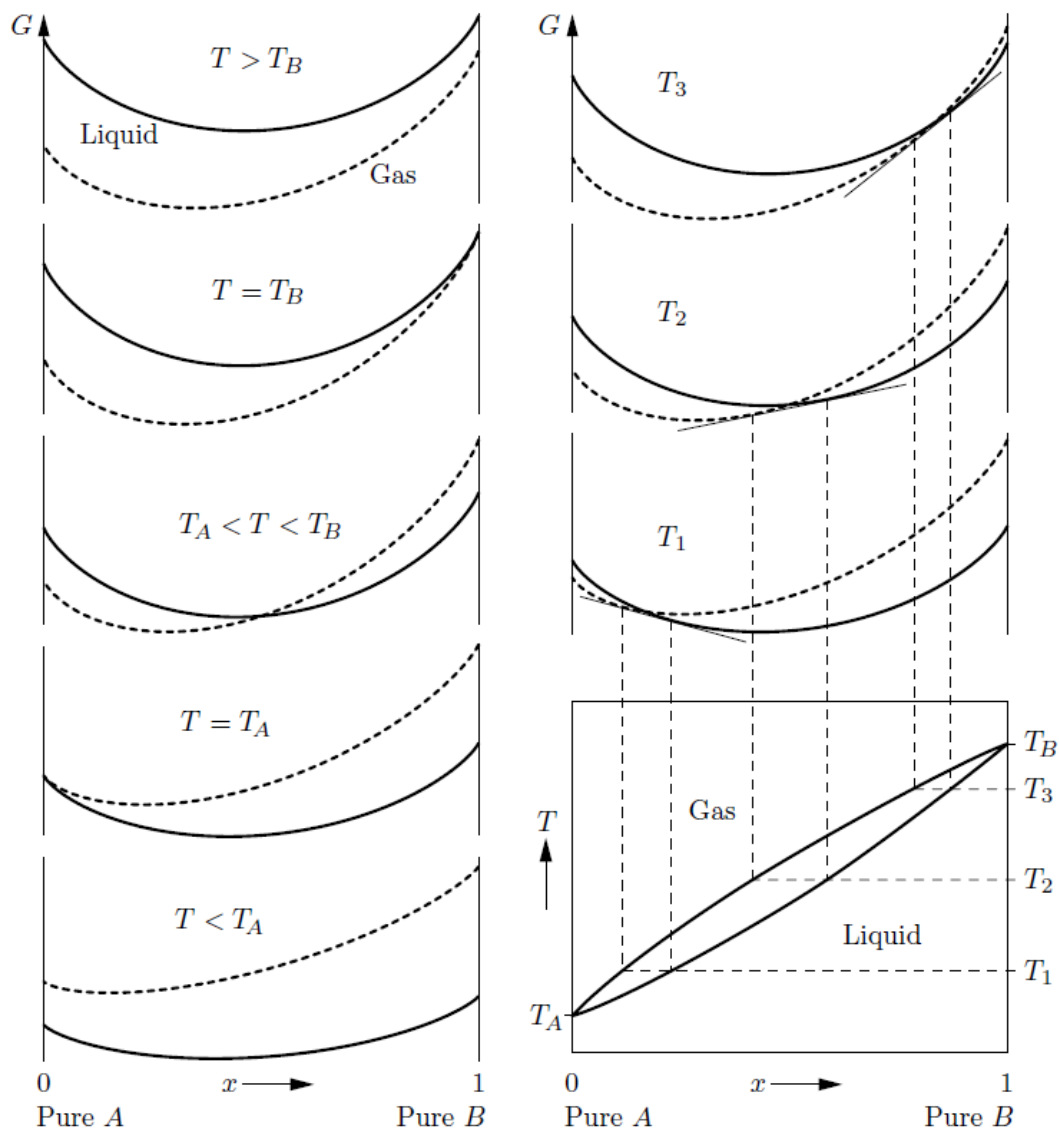


När kondenserar luft ?

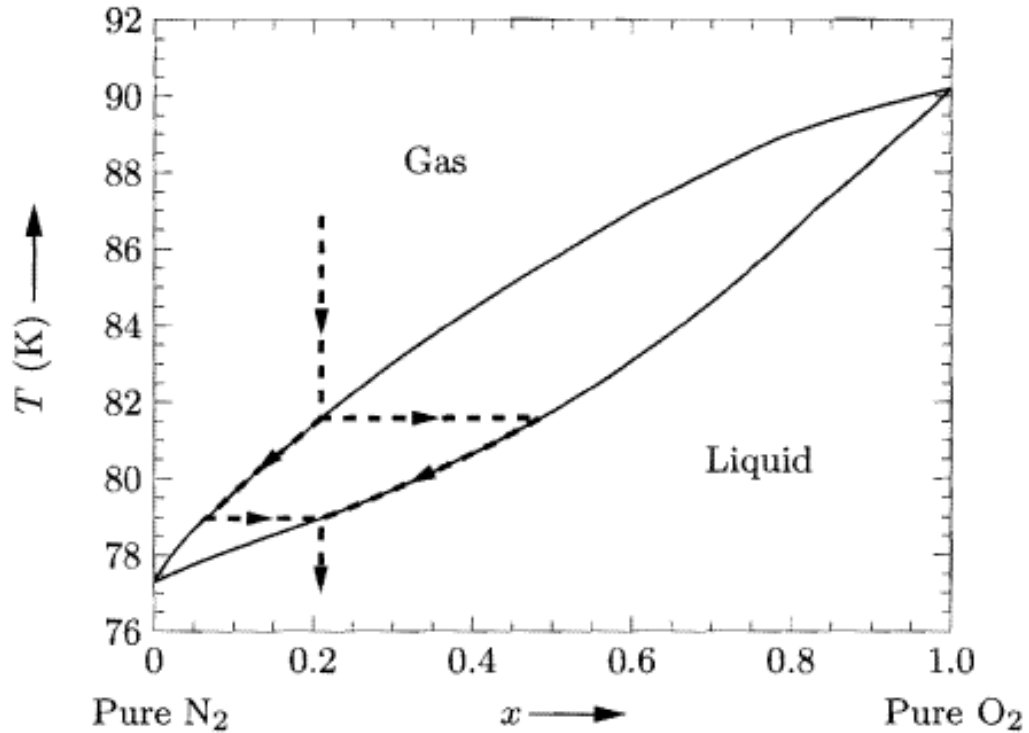
$$\text{N}_2 : T_K = 77.4 \text{ K}$$

$$\text{O}_2 : T_K = 90.2 \text{ K}$$

Fasdiagram för luft



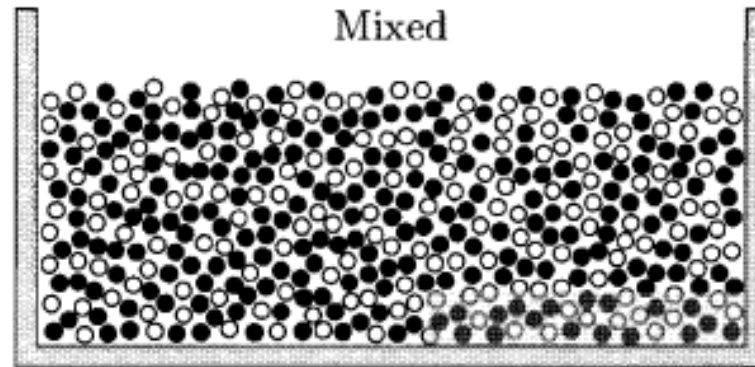
Experimentellt fasdiagramm för luft



$$N_2 : T_K = 77.4 \text{ K}$$

$$O_2 : T_K = 90.2 \text{ K}$$

Regulär blandning



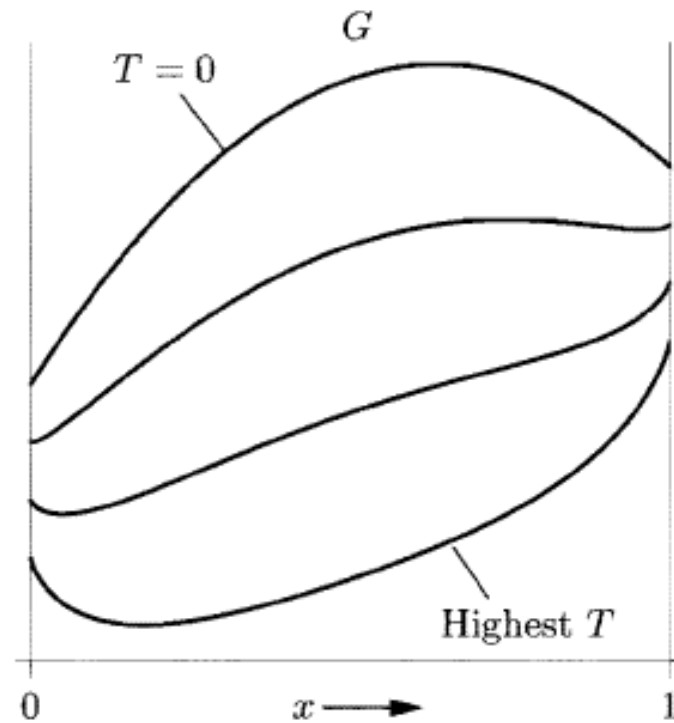
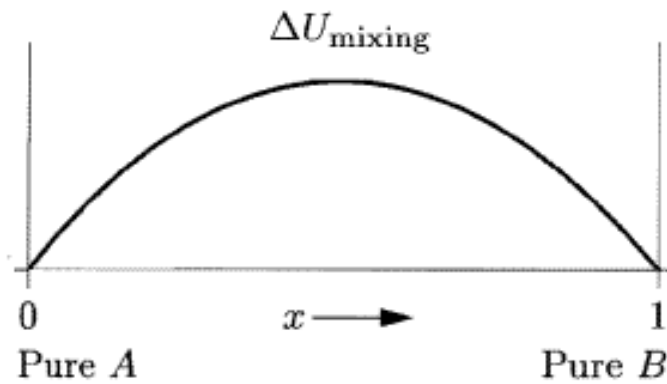
$$G = (1-x)G_A^o + xG_B^o + \Delta G_{mix}$$

$$\Delta G_{mix} = \Delta H_{mix} - T \Delta S_{mix}$$

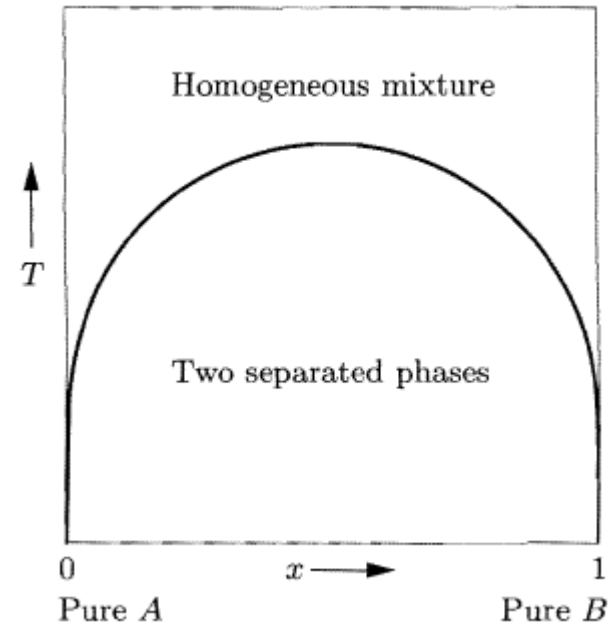
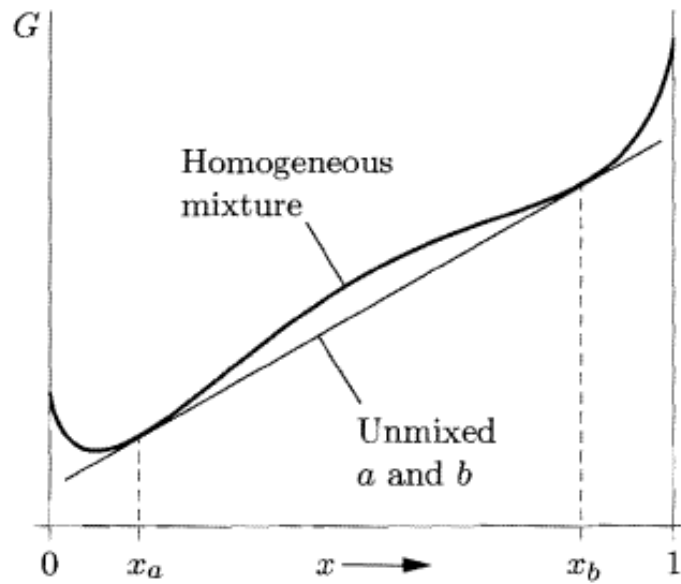
$$\Delta H_{mix} = Ax(1-x)$$

$$\Delta S_{mix} = -R[x \ln x + (1-x) \ln (1-x)]$$

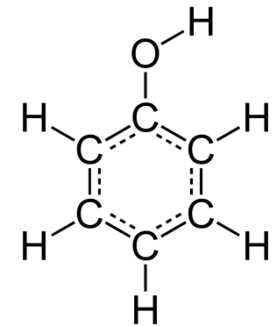
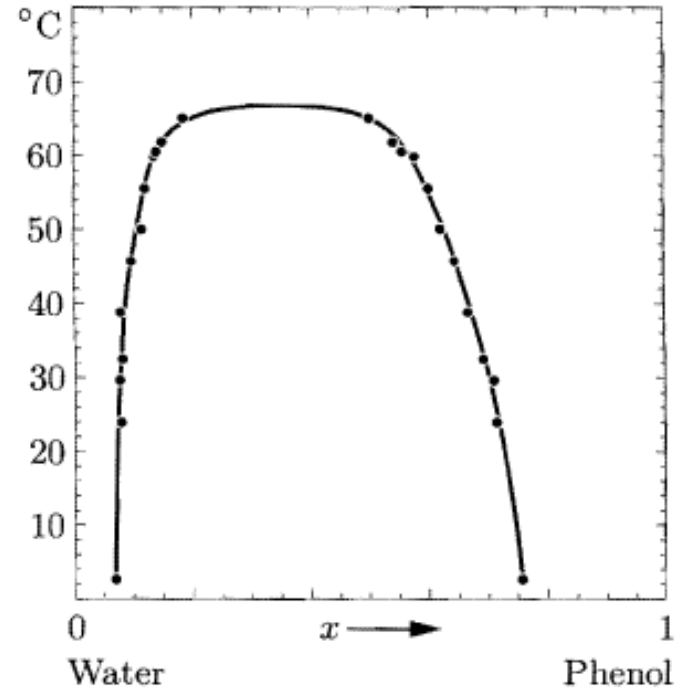
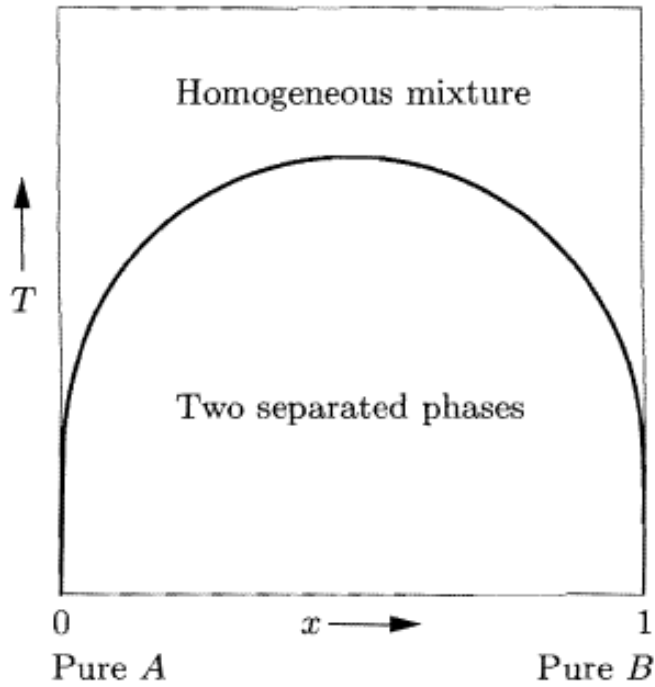
Regulär blandning



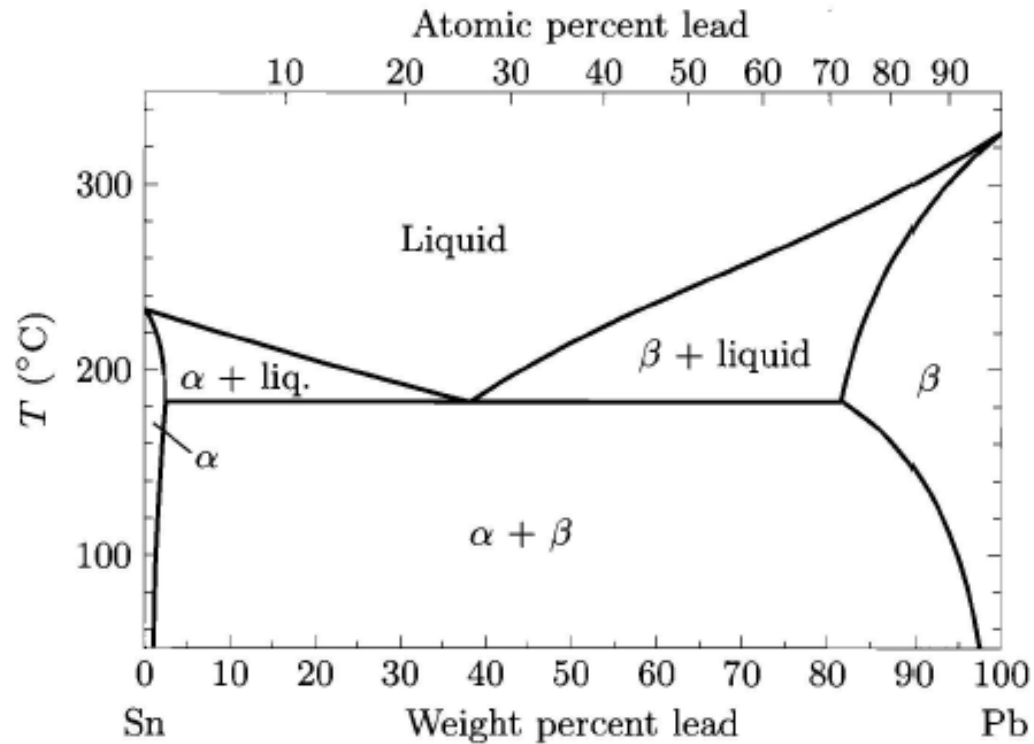
Regulär blandning - löslighetsgap



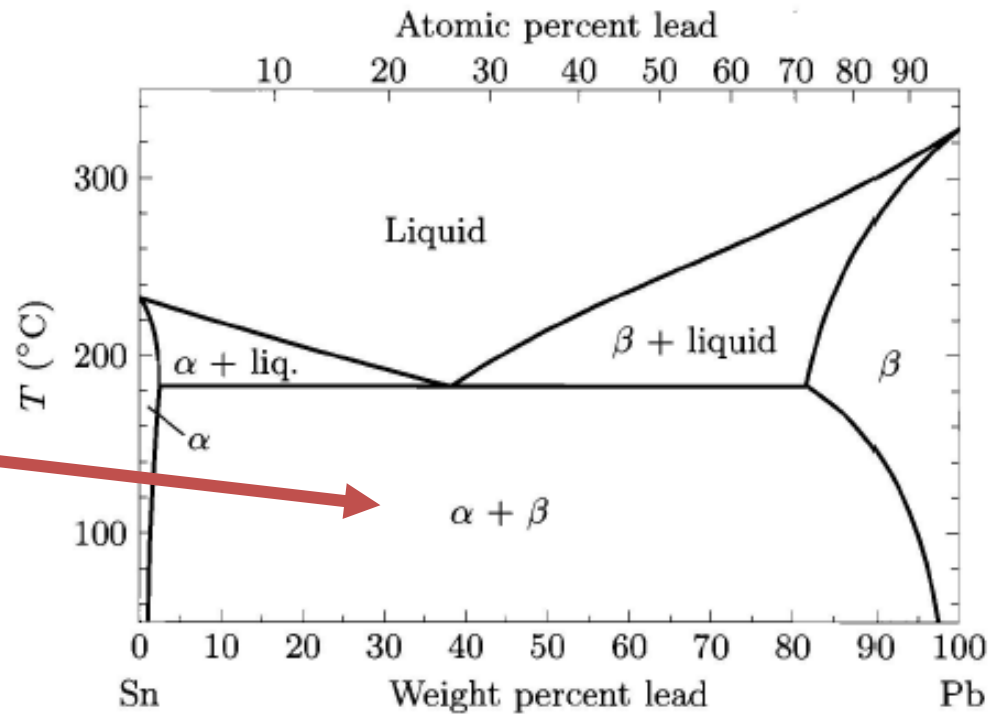
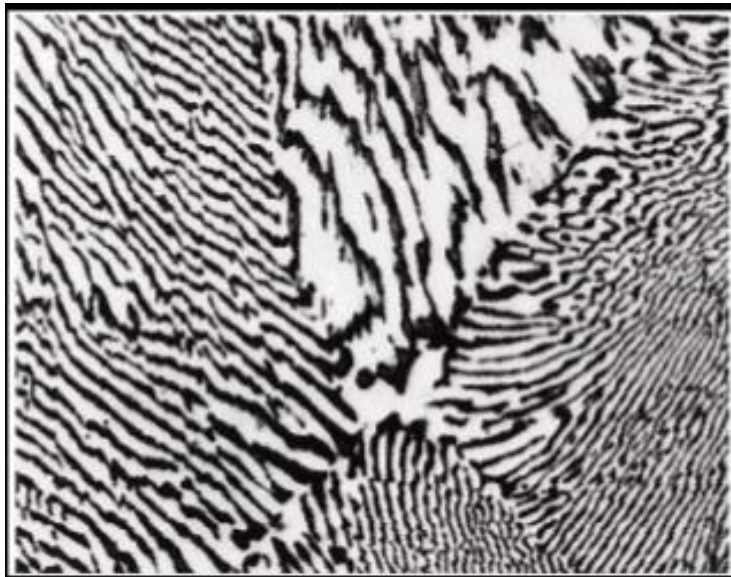
Regulär blandning - löslighetsgap



Eutektiska system



Eutektiska system

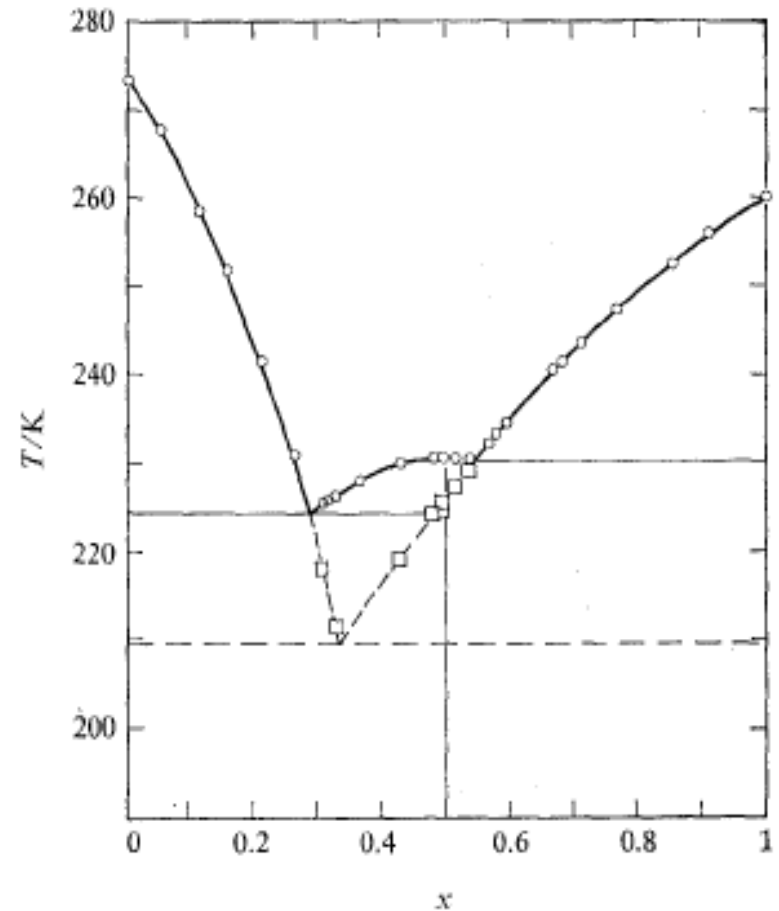


Vita områden är tenn(Sn)-rik alpha-fas
och svarta områden är bly(Pb)-rik beta-fas

När fryser kylarvätskan ?



Kylarvätska



J. Bevan Ott, J. Rex Goates, and John D. Lamb,
J. Chem. Thermodynamics 4, 123 (1972).

Kylarväska

Vatten:

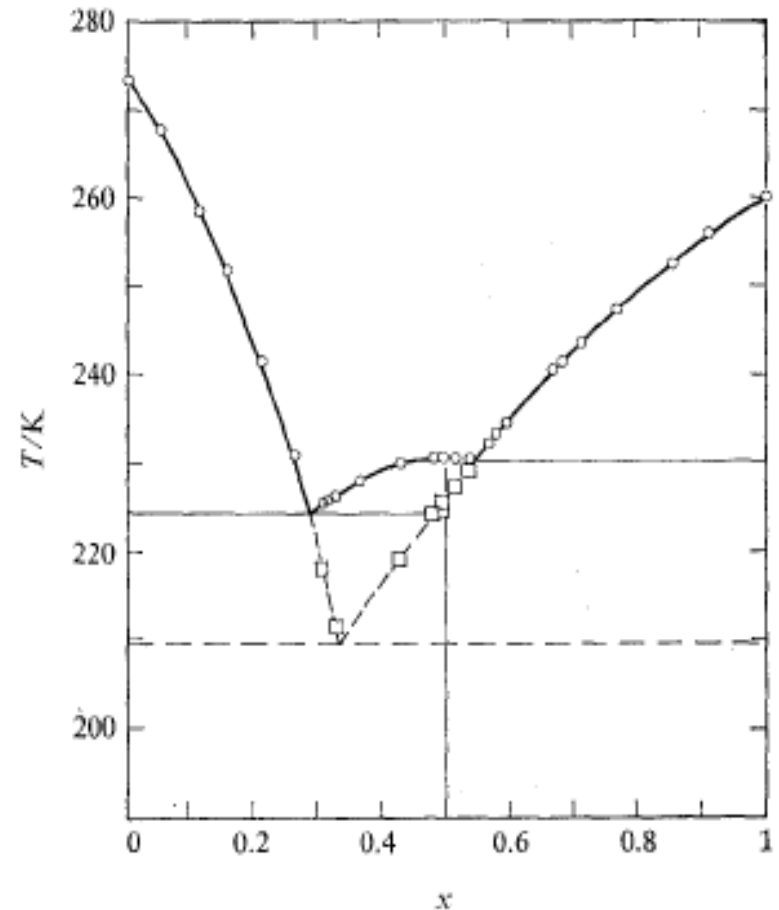
$$T_m = 0^\circ\text{C}$$

Glykol:

$$T_m = -13^\circ\text{C}$$

Kylarväska (vatten och glykol):

$$\min[T_m] = -49^\circ\text{C}$$



J. Bevan Ott, J. Rex Goates, and John D. Lamb,
J. Chem. Thermodynamics 4, 123 (1972).

Mikrotillstånd

Ett stort antal variabler

i) Kvantmekaniskt

$$\Psi(x_1, \dots, x_F)$$

ii) Klassiskt

$$q_1, \dots, q_F, p_1, \dots, p_F$$

$$F \sim 10^{23}$$

Mekanik

Statistisk



mekanik

Makrotillstånd

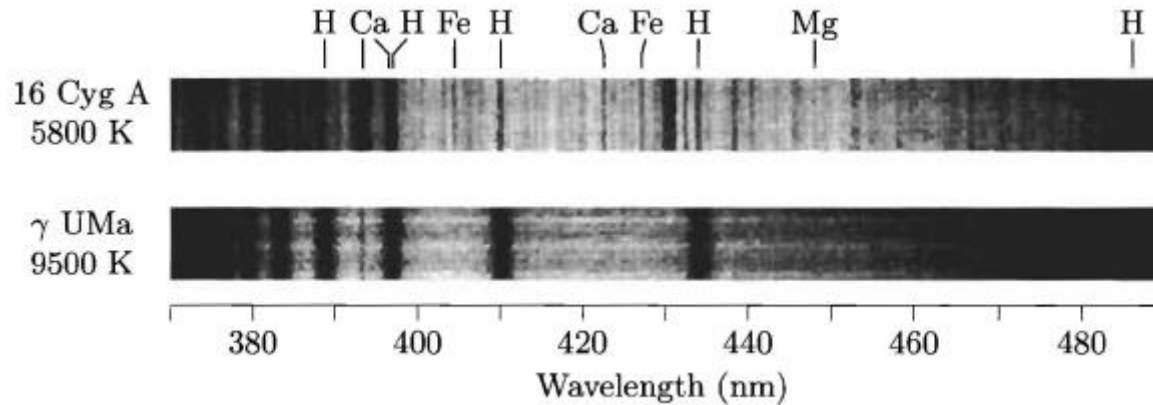
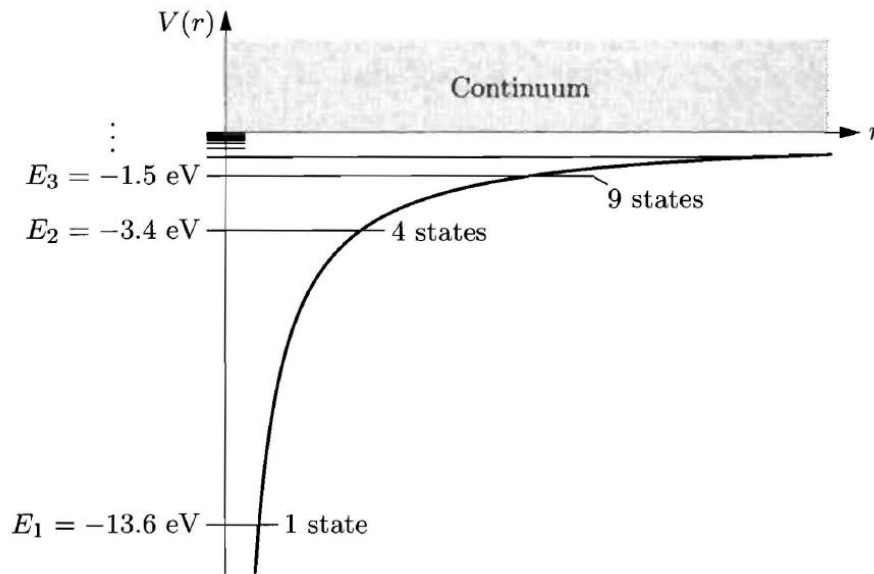
Ett fåtal variabler

Termodynamiska tillstånds-
variabler

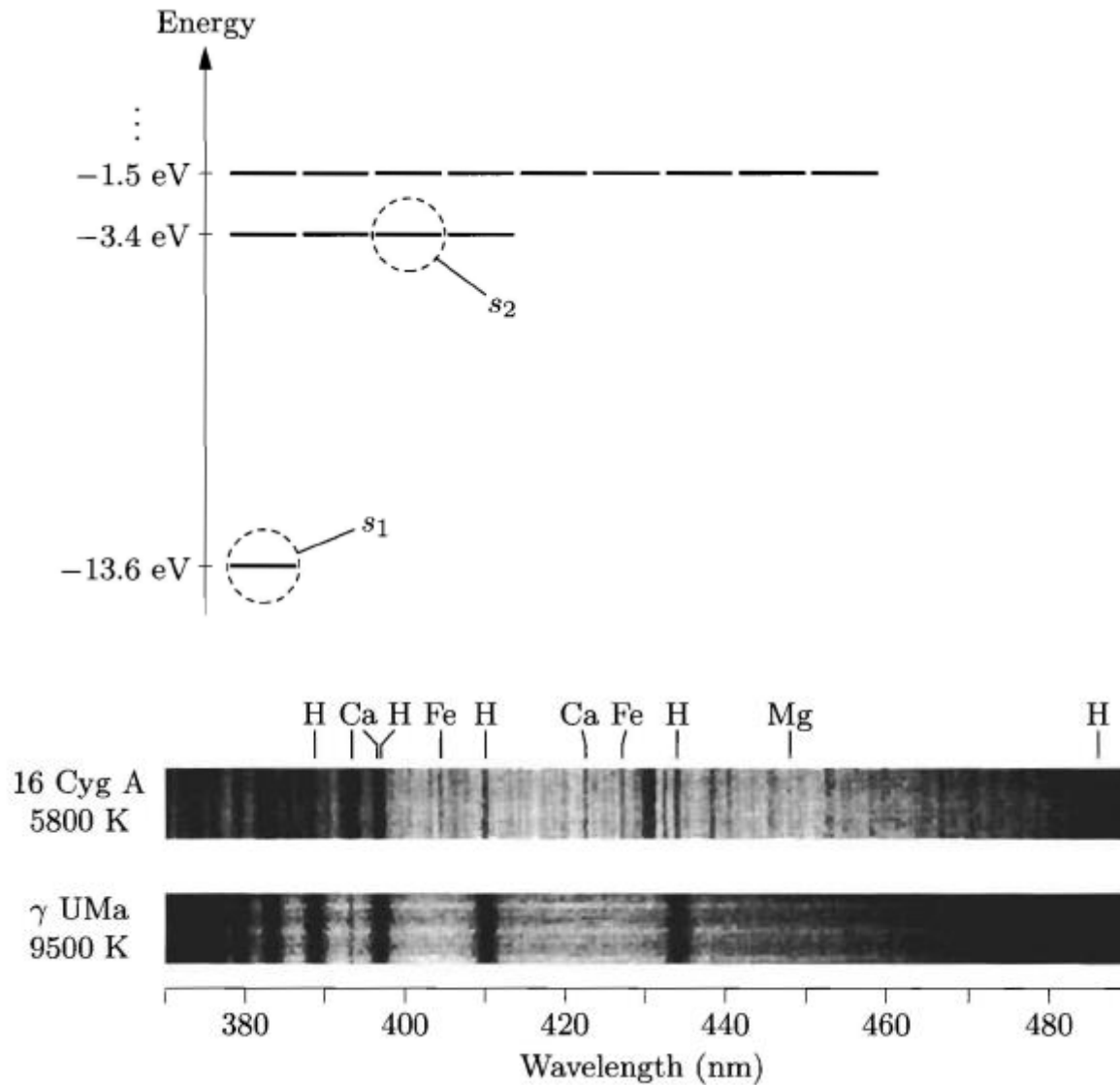
$$P, V, N, T, U, S, F, G \dots$$

Termodynamik

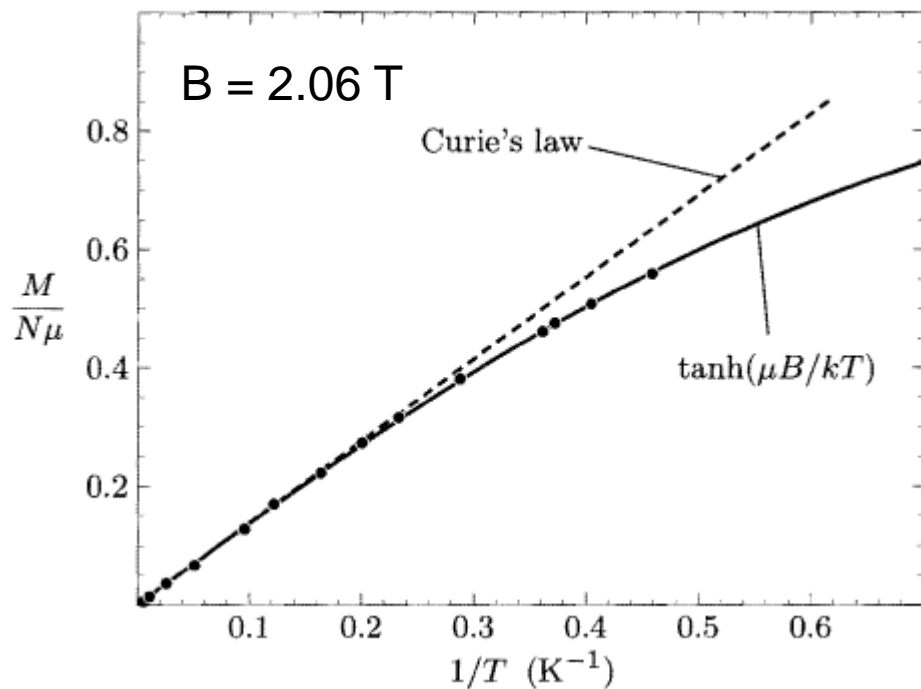
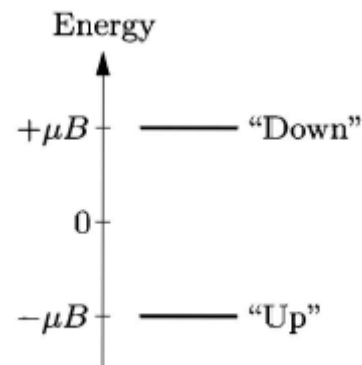
Väteatomerna



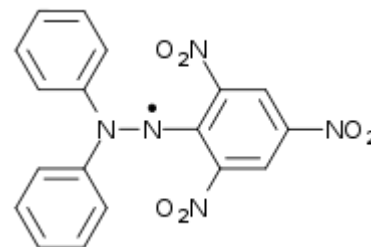
Väteatomerna



Paramagnetism

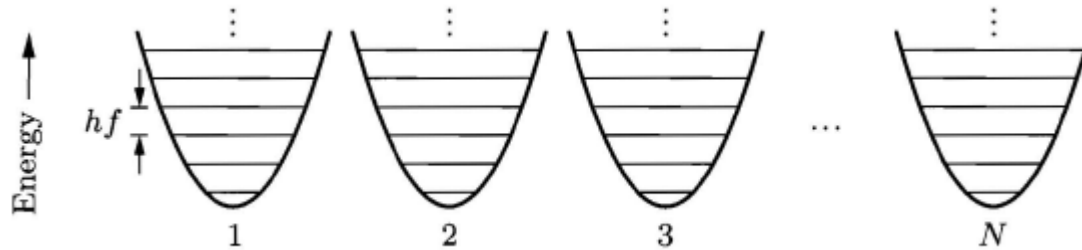


Experimentella data



P. Grobet et al,
J. Chem. Phys. **68**, 5225 (1978)

Harmoniska oscillatorer



Multipliciteten för en uppsättning av N identiska harmoniska oscillatorer ges av uttrycket

$$\Omega(N, q) = \frac{(q + N - 1)!}{q!(N - 1)!}$$

där q är totala antalet energikvanta för systemet,

$$E = qhf + E_0 ; \quad E_0 = (N/2)hf$$

Uttryck för stora system:

$$\begin{aligned} \Omega(N, q) &\rightarrow \left(\frac{q+N}{q}\right)^q \left(\frac{q+N}{N}\right)^N && \text{om } q, N \gg 1 \\ \Omega(N, q) &\rightarrow \left(\frac{eq}{N}\right)^N && \text{om } q \gg N \gg 1 \\ \Omega(N, q) &\rightarrow \left(\frac{eN}{q}\right)^q && \text{om } N \gg q \gg 1 \end{aligned}$$

Vibrerande molekyl

Klassisk beskrivning

$$E_{cl} = \frac{p^2}{2\mu} + \frac{k_s}{2}q^2 ; \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$\overline{E_{cl}} = 2 \frac{kT}{2}$$

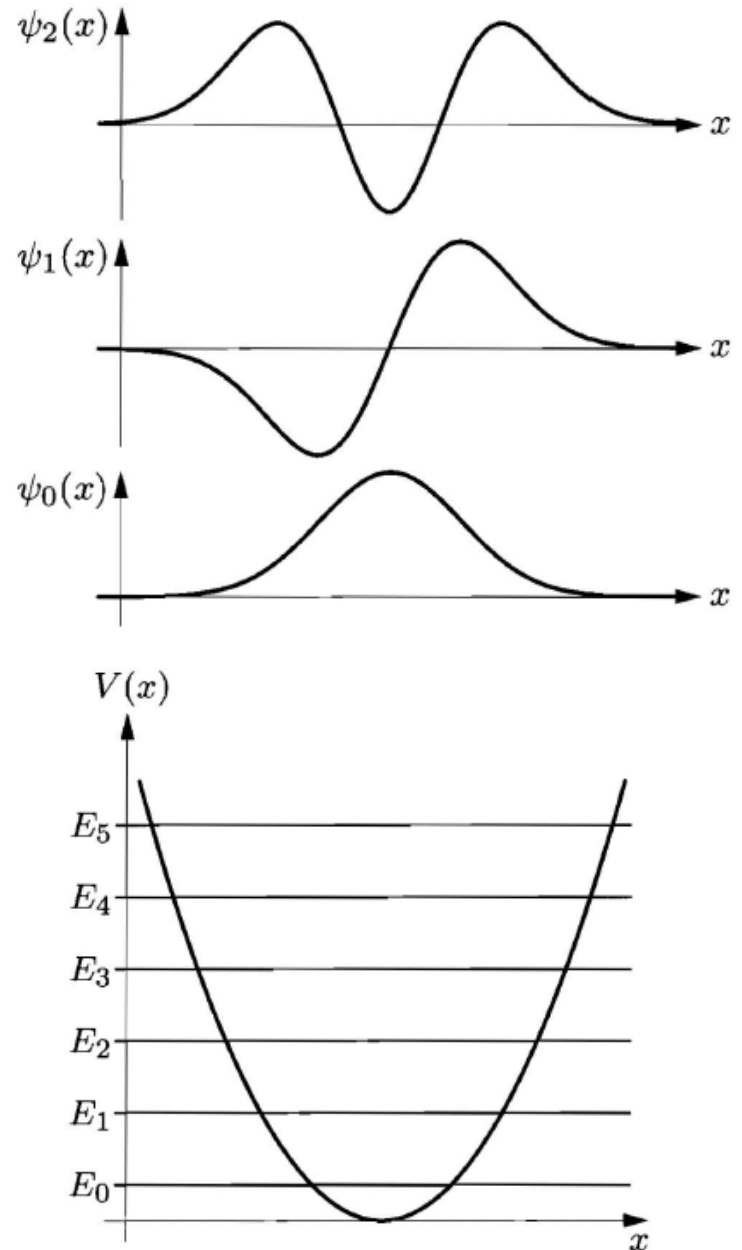
Kvantmekanisk beskrivning

$$E_n = \left(n + \frac{1}{2}\right)hf ; \quad f = \frac{1}{2\pi} \sqrt{\frac{k_s}{\mu}}$$

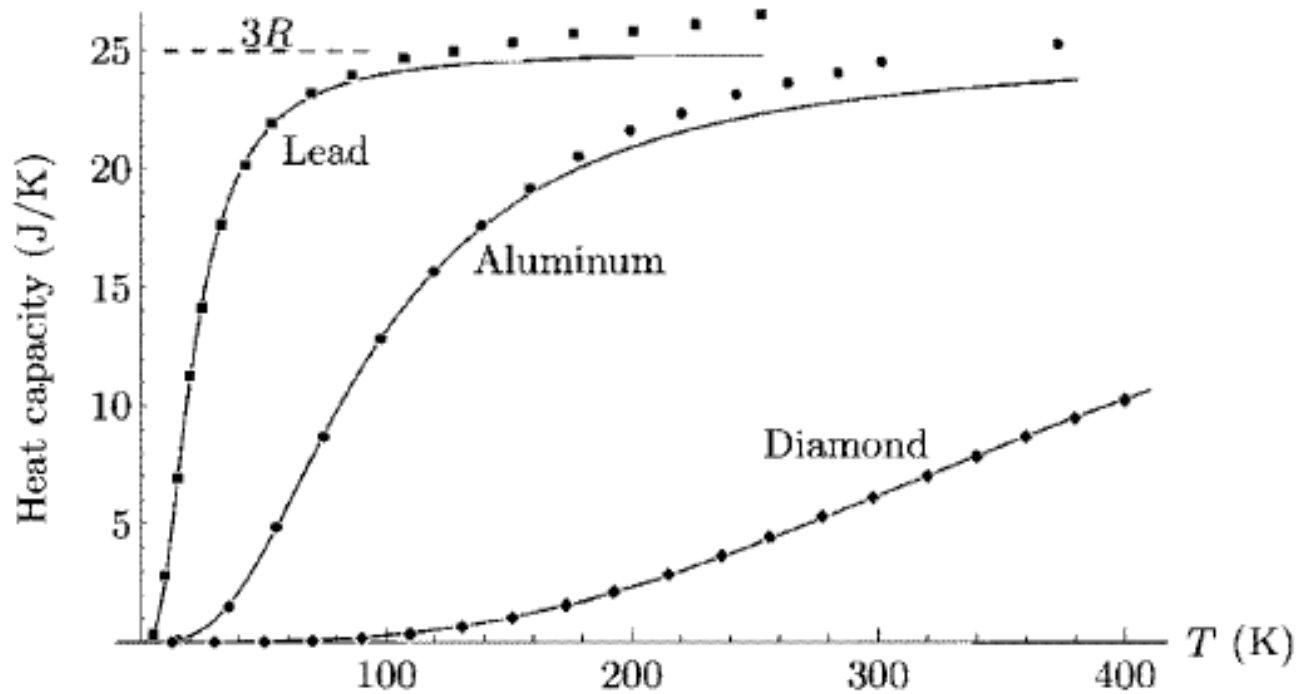
$$n = 0, 1, 2, \dots$$

Typisk energiuppsplittring

$$k\theta_{vib} \equiv hf$$



Vibrerande atomer i fasta material

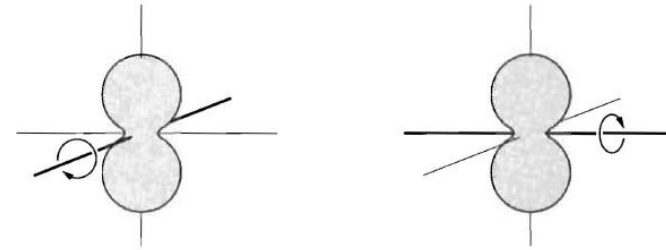


Roterande molekyl

Klassisk beskrivning

$$E_{cl} = \frac{1}{2I}(J_x^2 + J_y^2) ; \quad I = \mu R_0^2$$

$$\overline{E_{cl}} = 2 \frac{kT}{2}$$



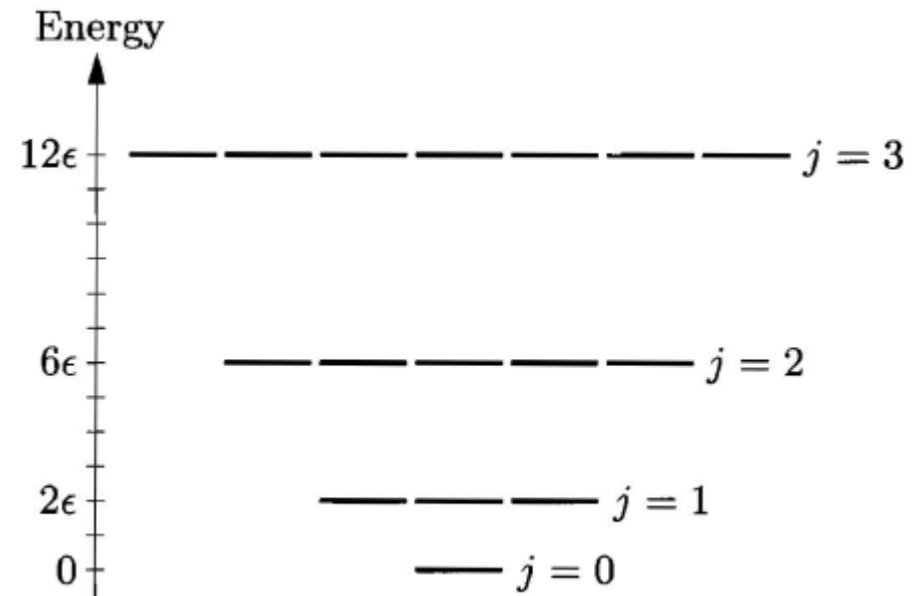
Kvantmekanisk beskrivning

$$E_j = \frac{\hbar^2}{2I}j(j+1) , \quad g_j = 2j+1$$

$$j = 0, 1, 2, \dots$$

Typisk energiuppsplittring

$$k\theta_{rot} \equiv \frac{\hbar^2}{2I}$$



Fri partikel i en låda

Klassisk beskrivning

$$E_{cl} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) = \frac{p^2}{2m}$$

$$\overline{E_{cl}} = 3 \frac{kT}{2}$$

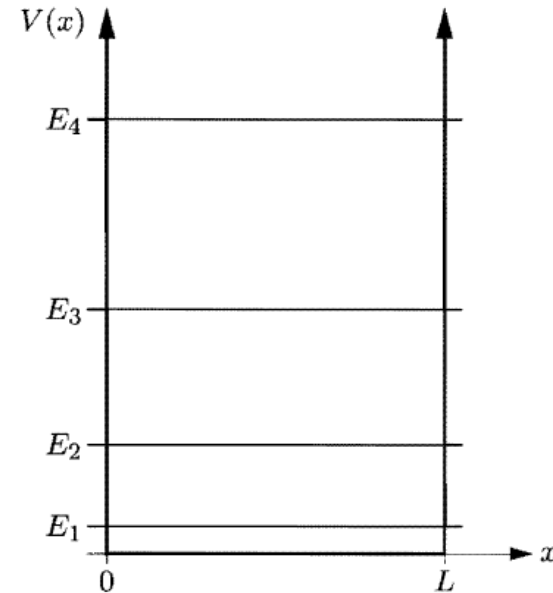
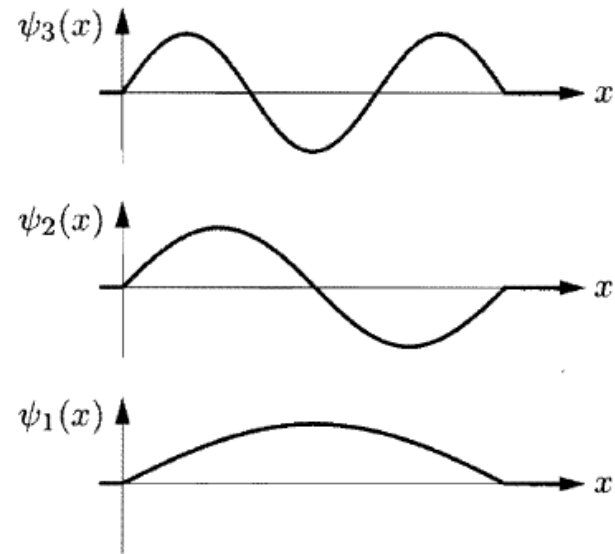
Kvantmekanisk beskrivning

$$E_{n_x n_y n_z} = \frac{1}{2m} \left(\frac{h}{2L} \right)^2 (n_x^2 + n_y^2 + n_z^2)$$

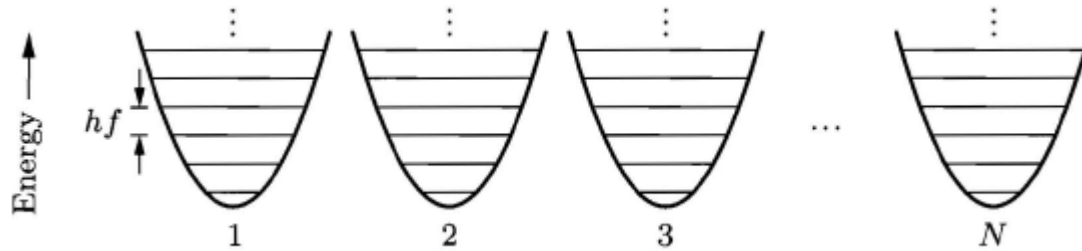
$$n_x, n_y, n_z \in \{1, 2, 3, \dots\}$$

Typisk energiuppsplittring

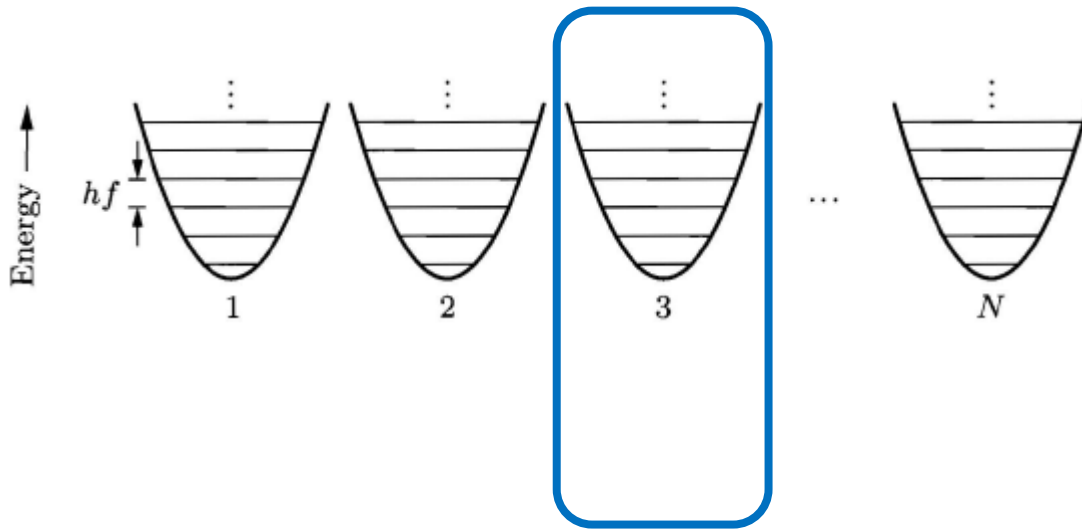
$$k\theta_{trans} \equiv \frac{1}{2m} \left(\frac{h}{2L} \right)^2$$



Harmoniska oscillatorer

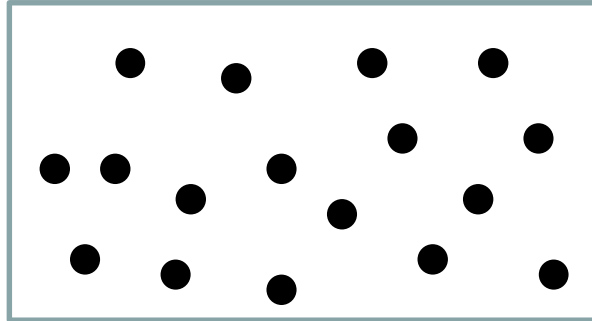


$$\Omega(N, q) = \frac{(q + N - 1)!}{q!(N - 1)!}$$



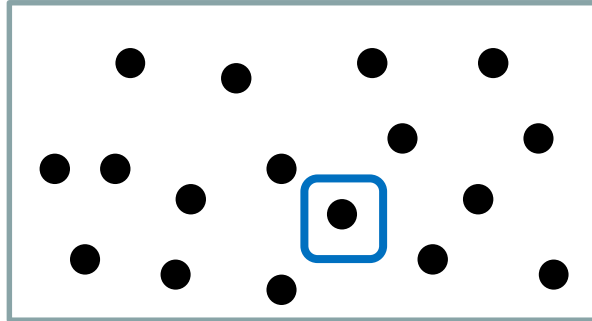
Vårt system

Klassisk idealgas

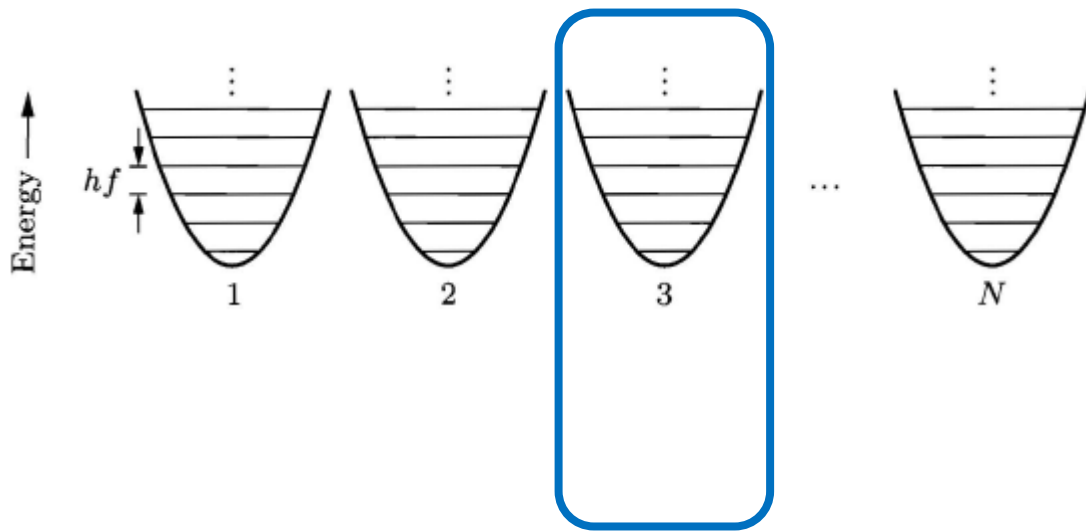


$$\Omega(N, V, U) = \frac{1}{N!} \frac{\pi^{3N/2}}{(3N/2)!} \frac{V^N}{h^{3N}} (2mU)^{3N/2} \equiv f(N) V^N U^{3N/2}$$

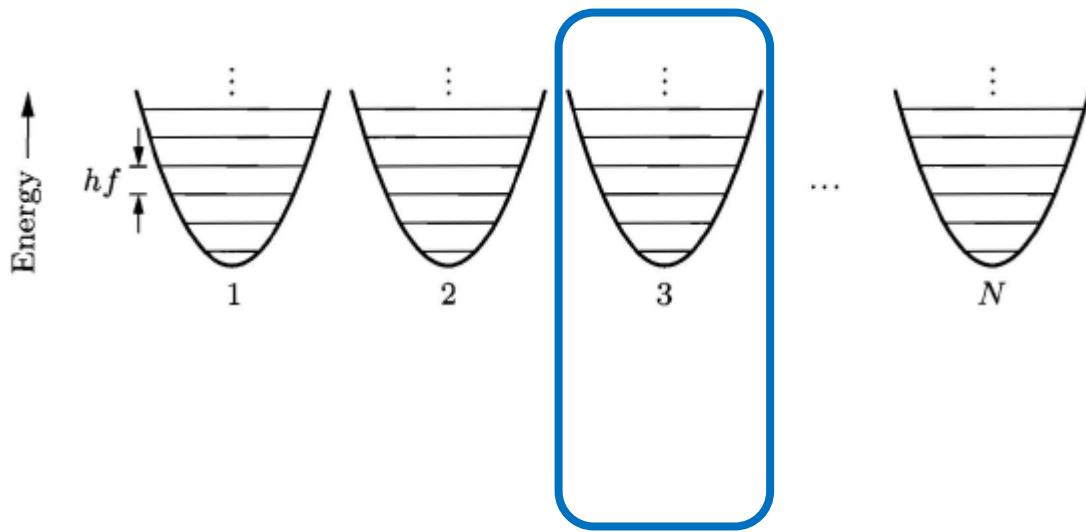
Klassisk idealgas



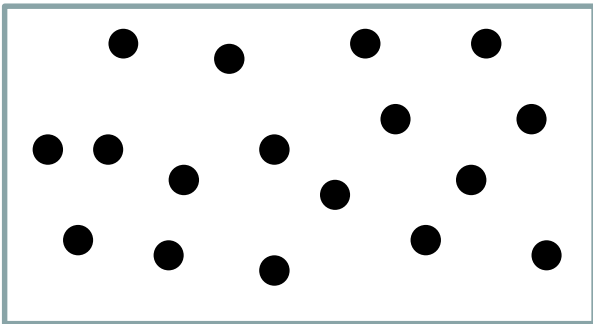
Vårt system

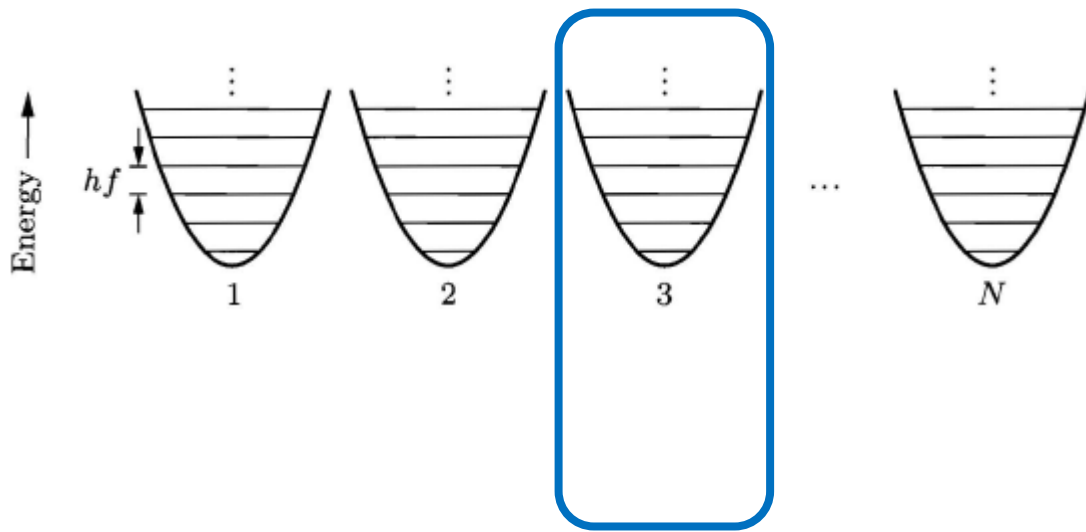


Vårt system

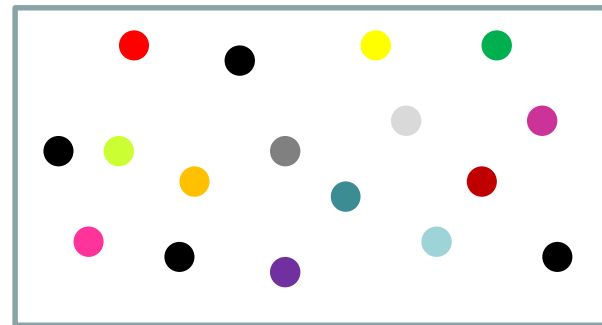
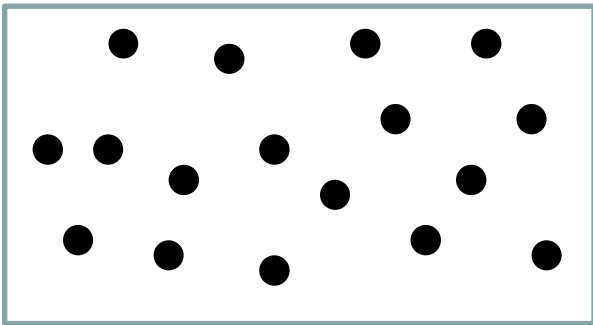


Vårt system



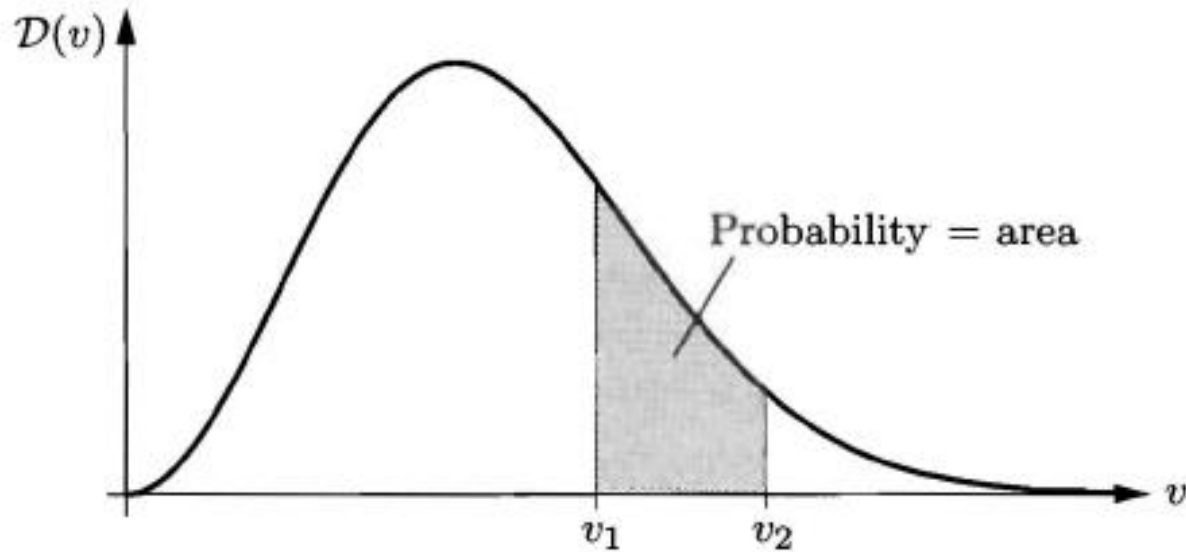


Vårt system



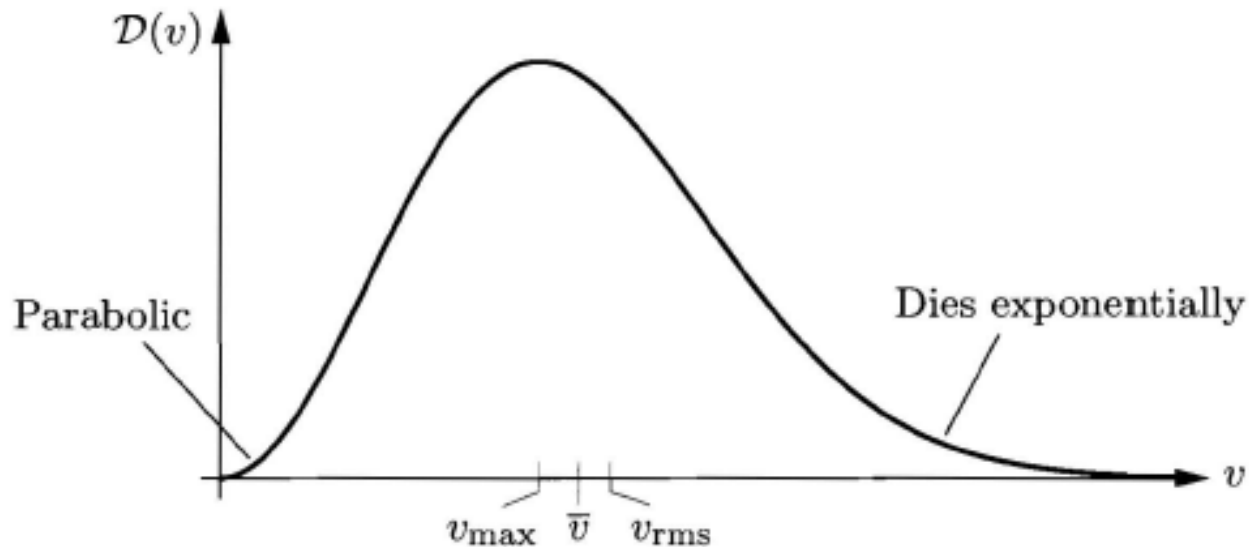
Maxwells hastighets(fart)fördelning

$$D(v) = \left(\frac{m}{2\pi kT} \right)^{3/2} 4\pi v^2 e^{-mv^2/2kT}$$



Maxwells hastighets(fart)fördelning

$$D(v) = \left(\frac{m}{2\pi kT}\right)^{3/2} 4\pi v^2 e^{-mv^2/2kT}$$

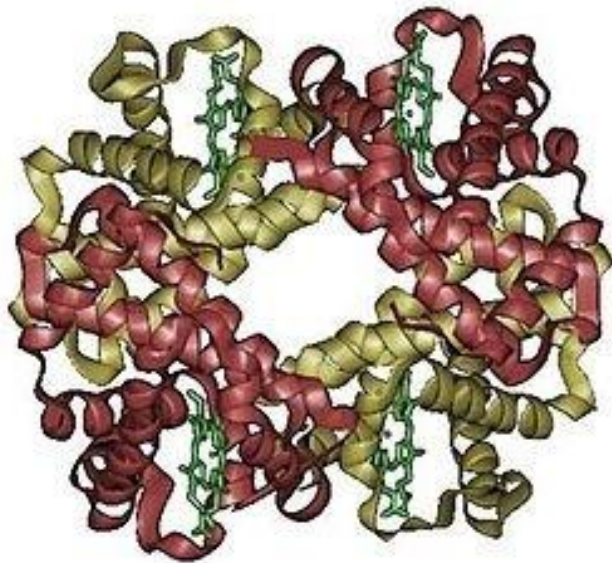


$$v_{\max} = \sqrt{2} \sqrt{\frac{kT}{m}}$$

$$\bar{v} = \sqrt{\frac{8}{\pi}} \sqrt{\frac{kT}{m}}$$

$$v_{\text{rms}} = \sqrt{3} \sqrt{\frac{kT}{m}}$$

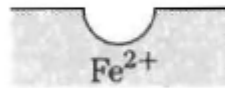
Hur blir man koloxidförgiftad ?



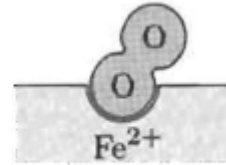
Kan vi förstå egenskaperna för elektroner i en metall ?



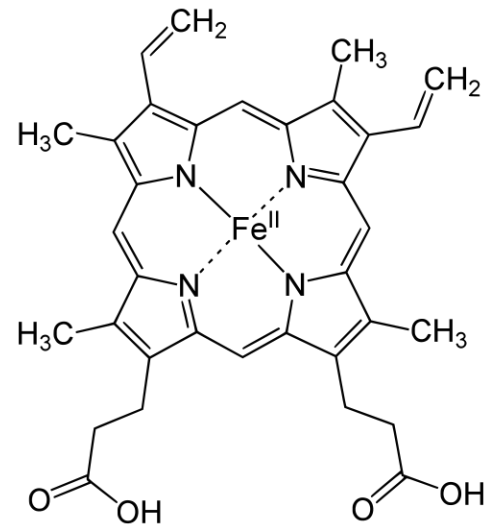
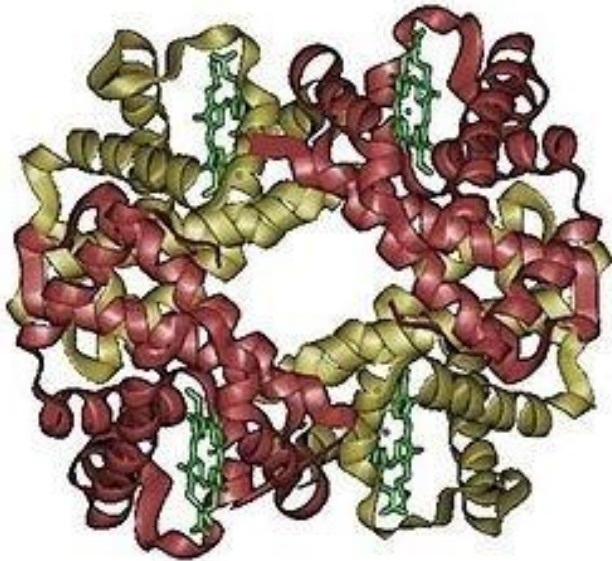
Hemoglobin



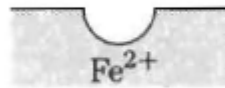
$$E = 0$$



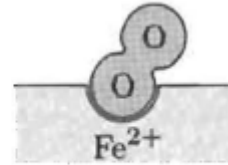
$$E = -0.7 \text{ eV}$$



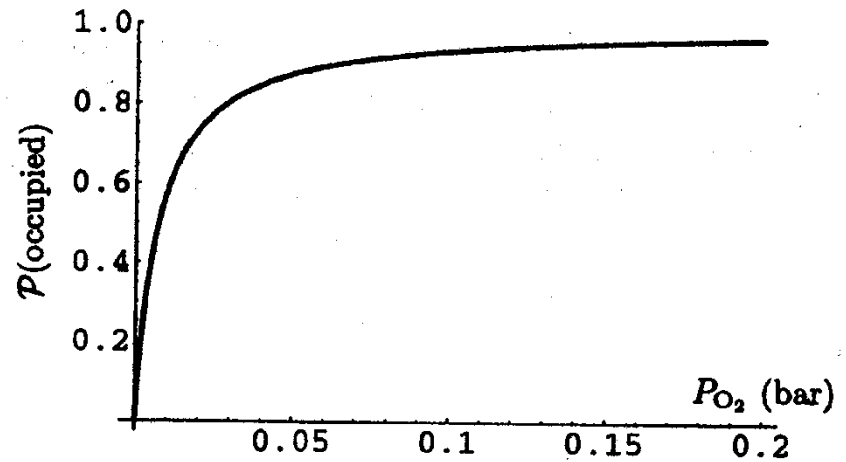
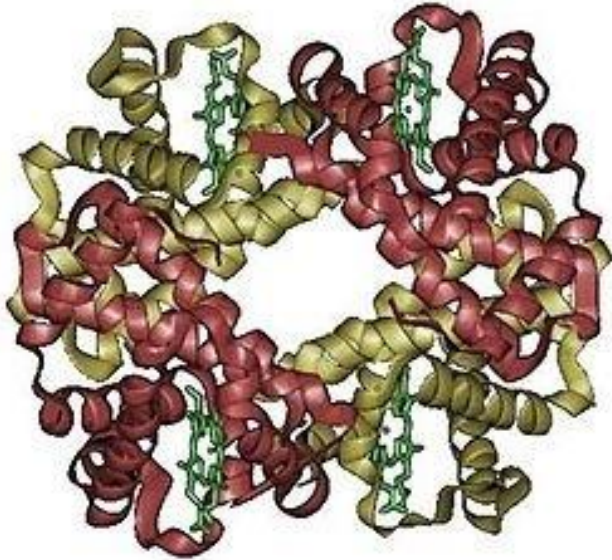
Hemoglobin



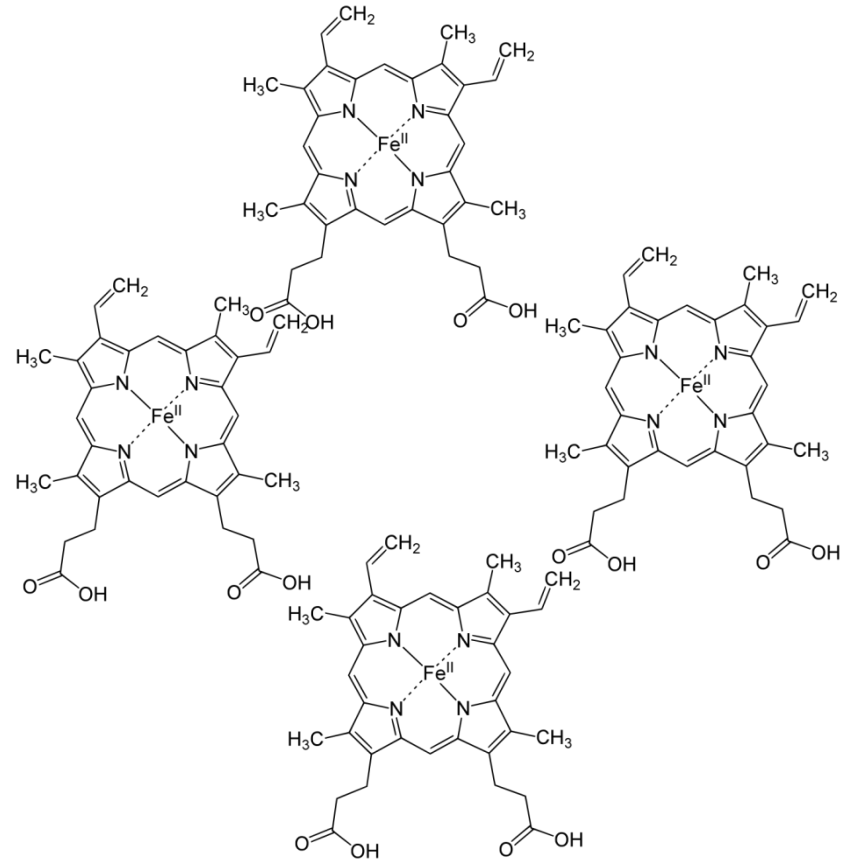
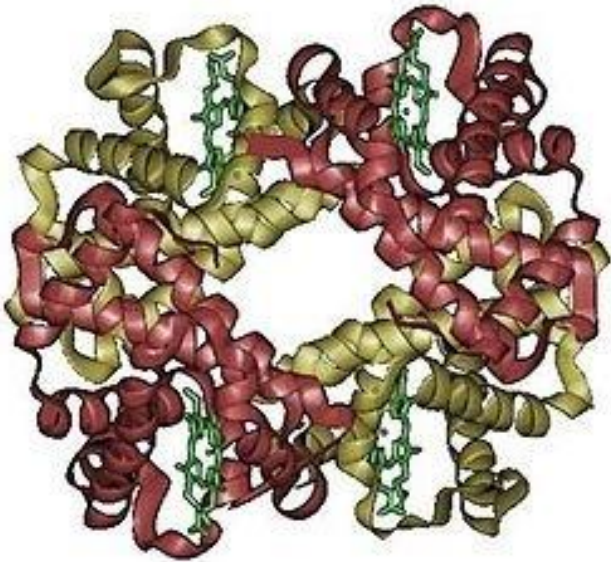
$$E = 0$$



$$E = -0.7 \text{ eV}$$

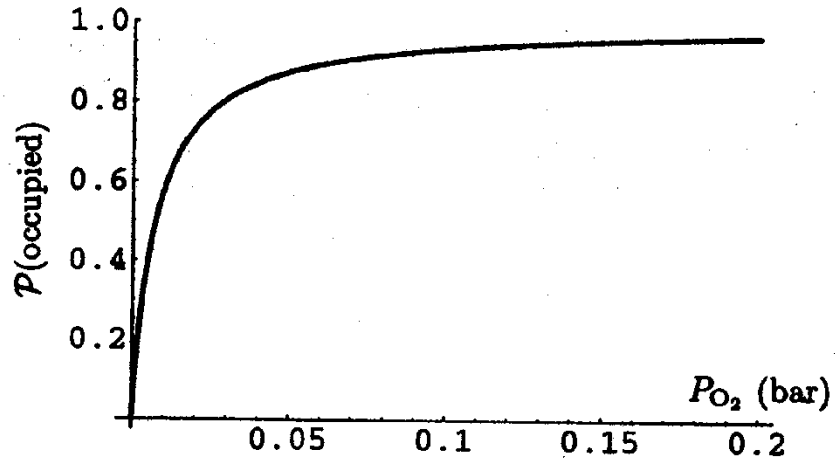


Hemoglobin



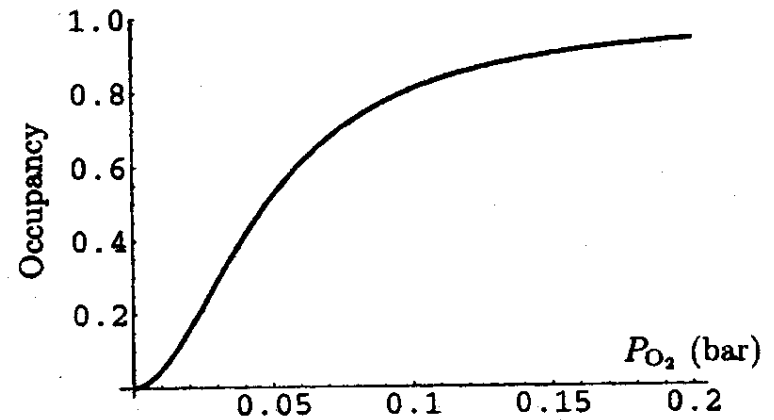
Hemoglobin

1 Fe-plats



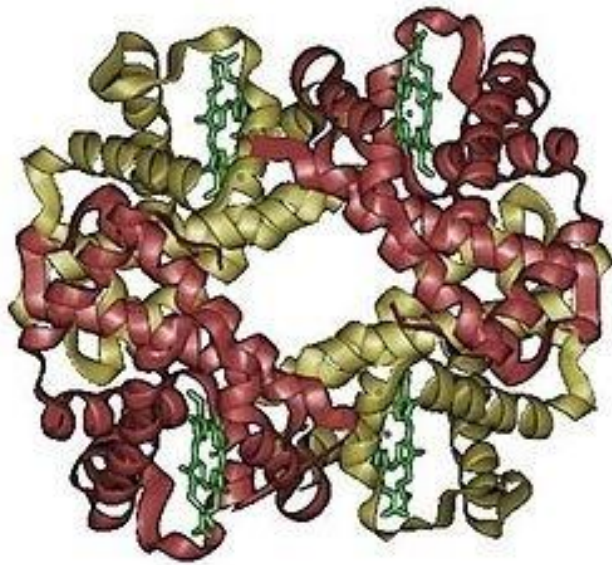
Uppg 7.1

4 Fe-platser

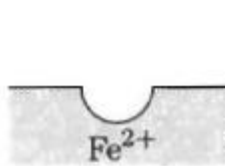


Uppg 7.2

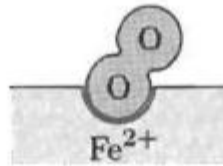
Hur blir man koloxidförgiftad ?



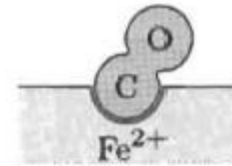
Hemoglobin



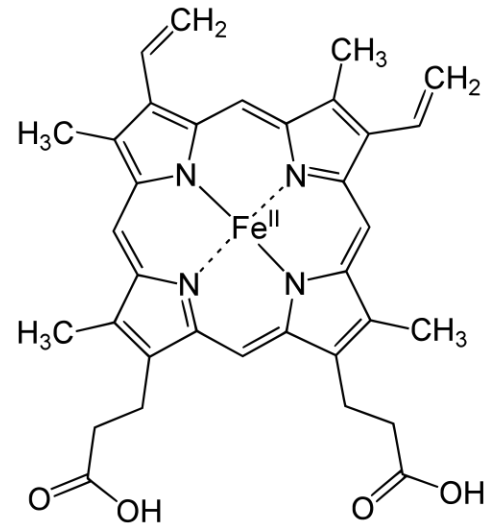
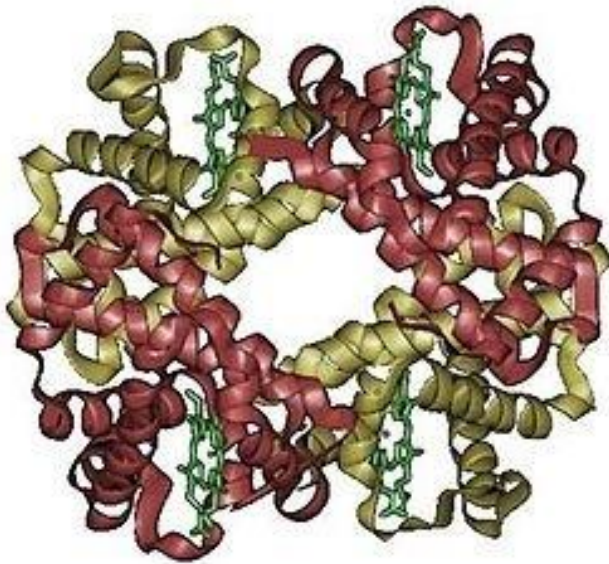
$$E = 0$$



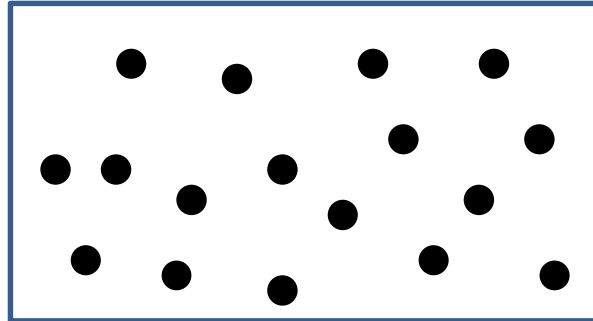
$$E = -0.7 \text{ eV}$$



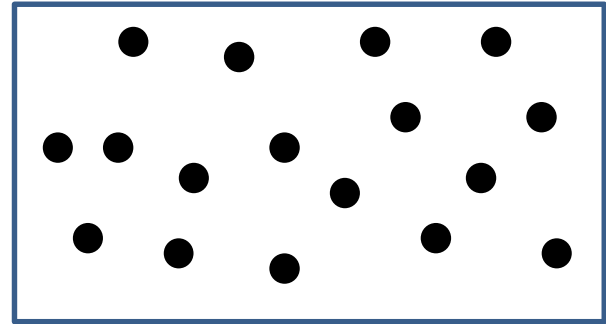
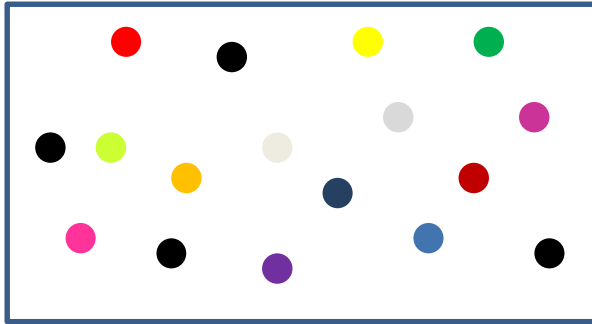
$$E = -0.85 \text{ eV}$$



Idealgas – icke-växelverkande partiklar



Idealgas – icke-växelverkande partiklar



Fri partikel i en låda

Klassisk beskrivning

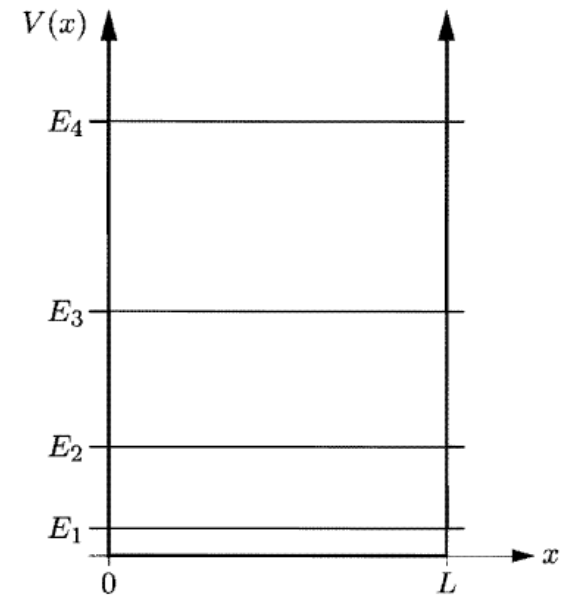
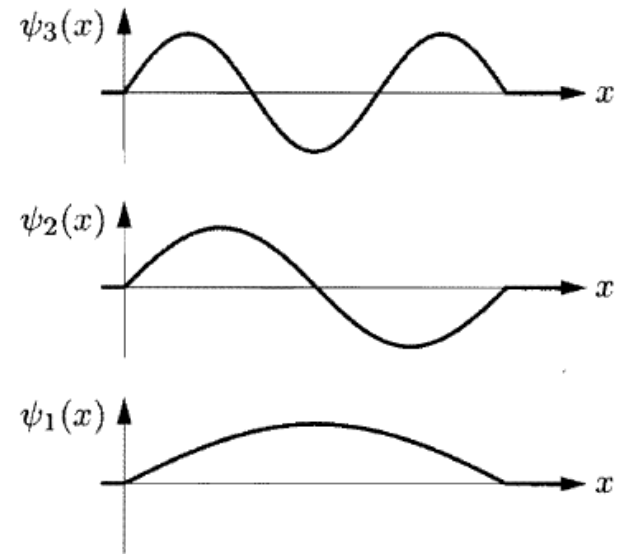
$$E_{cl} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) = \frac{p^2}{2m}$$

$$\overline{E_{cl}} = 3 \frac{kT}{2}$$

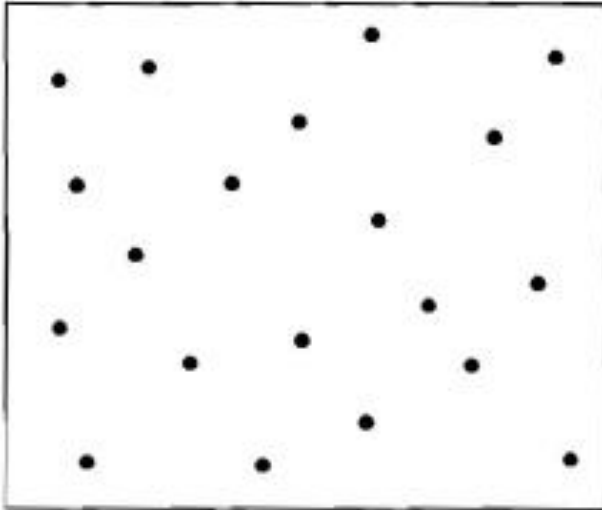
Kvantmekanisk beskrivning

$$E_{n_x n_y n_z} = \frac{1}{2m} \left(\frac{h}{2L} \right)^2 (n_x^2 + n_y^2 + n_z^2)$$

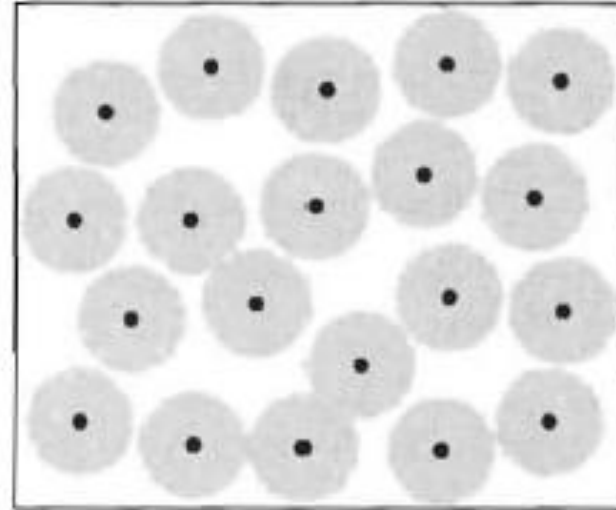
$$n_x, n_y, n_z \in \{1, 2, 3, \dots\}$$



Klassisk \leftrightarrow Kvant-idealgas

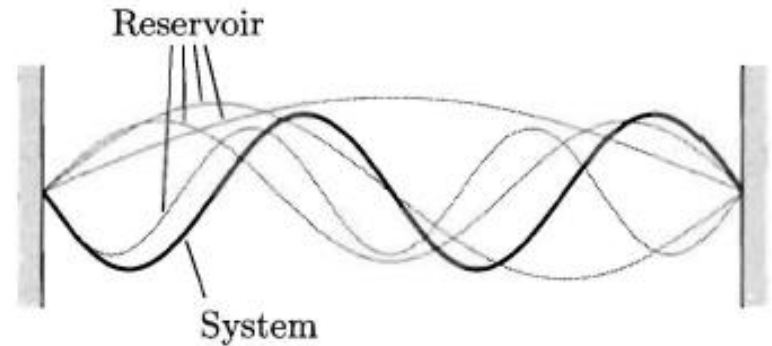
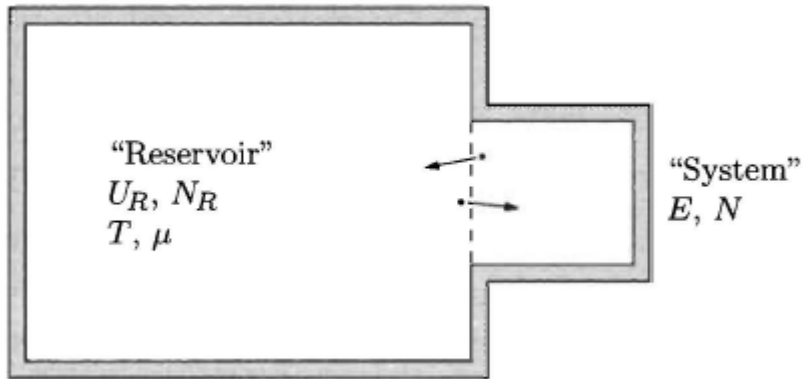


Normal gas, $V/N \gg v_Q$



Quantum gas, $V/N \approx v_Q$

En-partikel tillstånd



$$\mathcal{P}(s) = \frac{1}{\mathcal{Z}} e^{-[E(s) - \mu N(s)]/kT}$$

$$\mathcal{Z} \equiv \sum_s e^{-[E(s) - \mu N(s)]/kT}$$

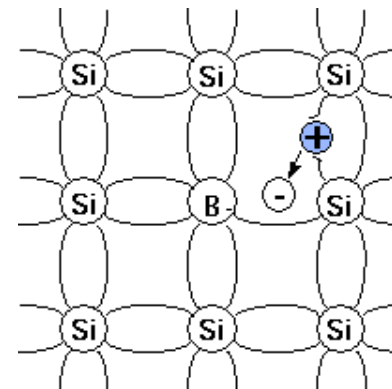
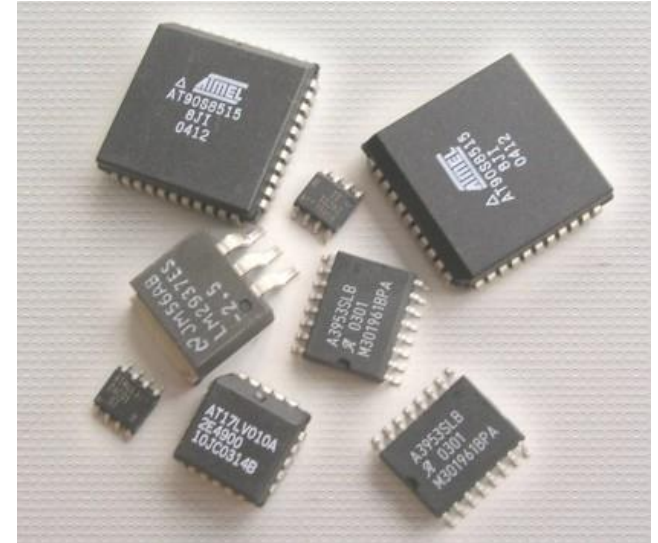
Kan vi förstå egenskaperna för
elektroner i en metall ?



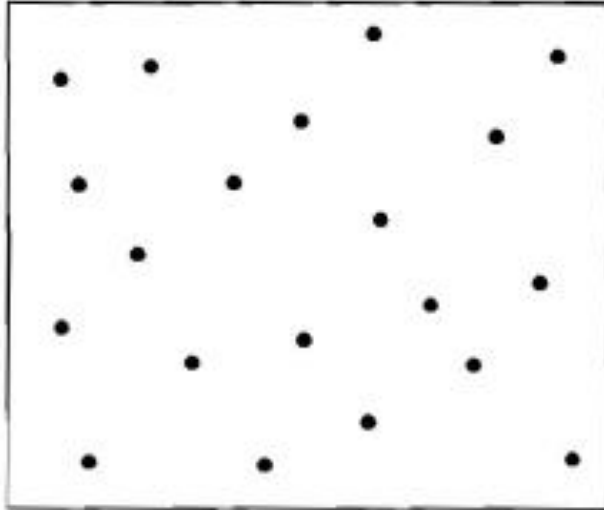
Kan vi förstå stabiliteten av
stjärnor ?



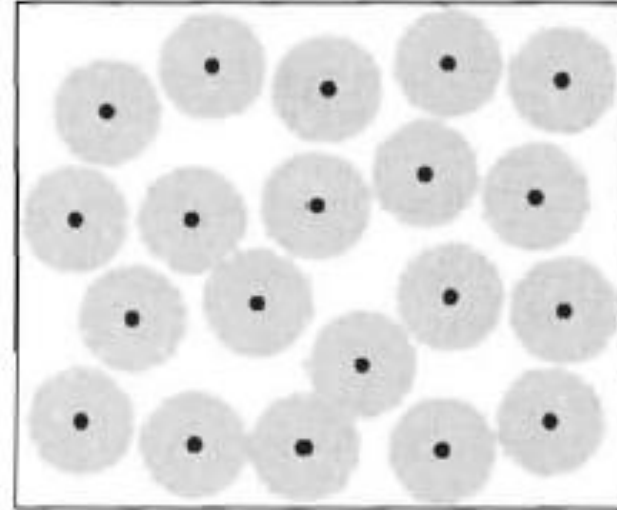
Vad händer när man dopar
halvledare ?



Klassisk \leftrightarrow Kvant-idealgas



Normal gas, $V/N \gg v_Q$



Quantum gas, $V/N \approx v_Q$

Kan vi förstå egenskaperna för
elektroner i en metall ?

Egenskaper vid 300 K

$$l_Q \sim 4.3 \text{ nm}$$

$$l \sim 0.23 \text{ nm}$$



Kan vi förstå egenskaperna för
elektroner i en metall ?

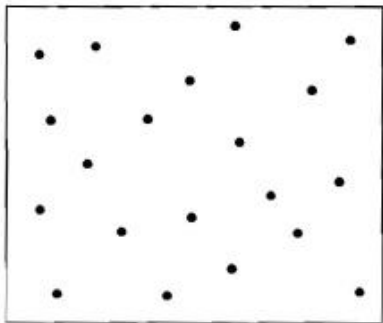
Egenskaper vid 300 K

$$l_Q \sim 4.3 \text{ nm}$$

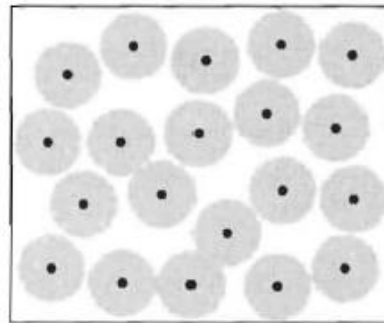
$$l \sim 0.23 \text{ nm}$$

$$l \ll l_Q$$

$$V/N \ll v_Q$$



Normal gas, $V/N \gg v_Q$



Quantum gas, $V/N \approx v_Q$



Fri partikel i en låda

Klassisk beskrivning

$$E_{cl} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) = \frac{p^2}{2m}$$

$$\overline{E_{cl}} = 3 \frac{kT}{2}$$

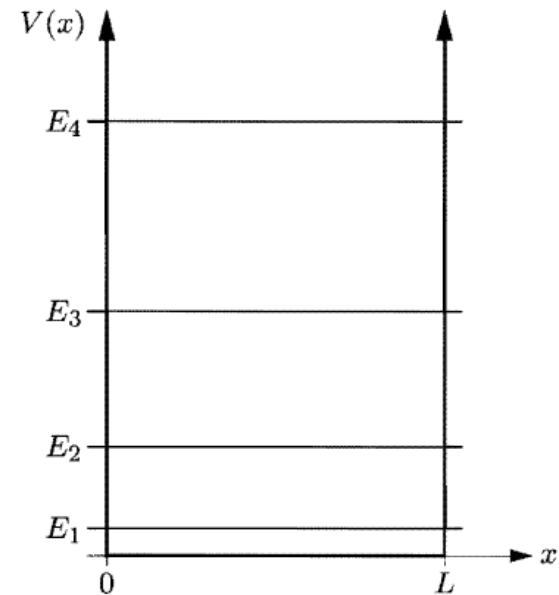
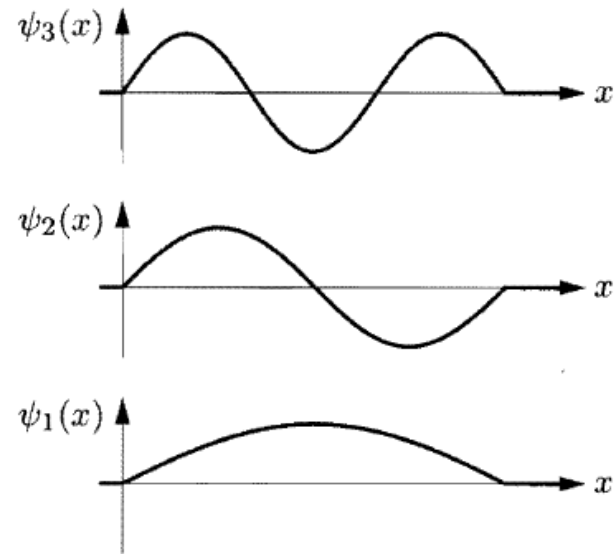
Kvantmekanisk beskrivning

$$E_{n_x n_y n_z} = \frac{1}{2m} \left(\frac{h}{2L} \right)^2 (n_x^2 + n_y^2 + n_z^2)$$

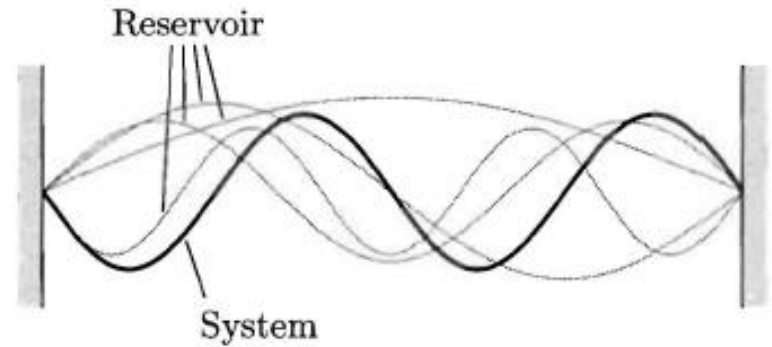
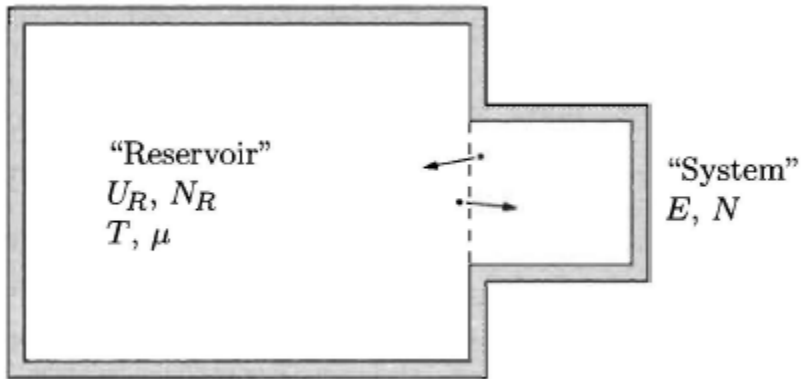
$$n_x, n_y, n_z \in \{1, 2, 3, \dots\}$$

Typisk energiuppsplittring

$$k\theta_{trans} \equiv \frac{1}{2m} \left(\frac{h}{2L} \right)^2$$



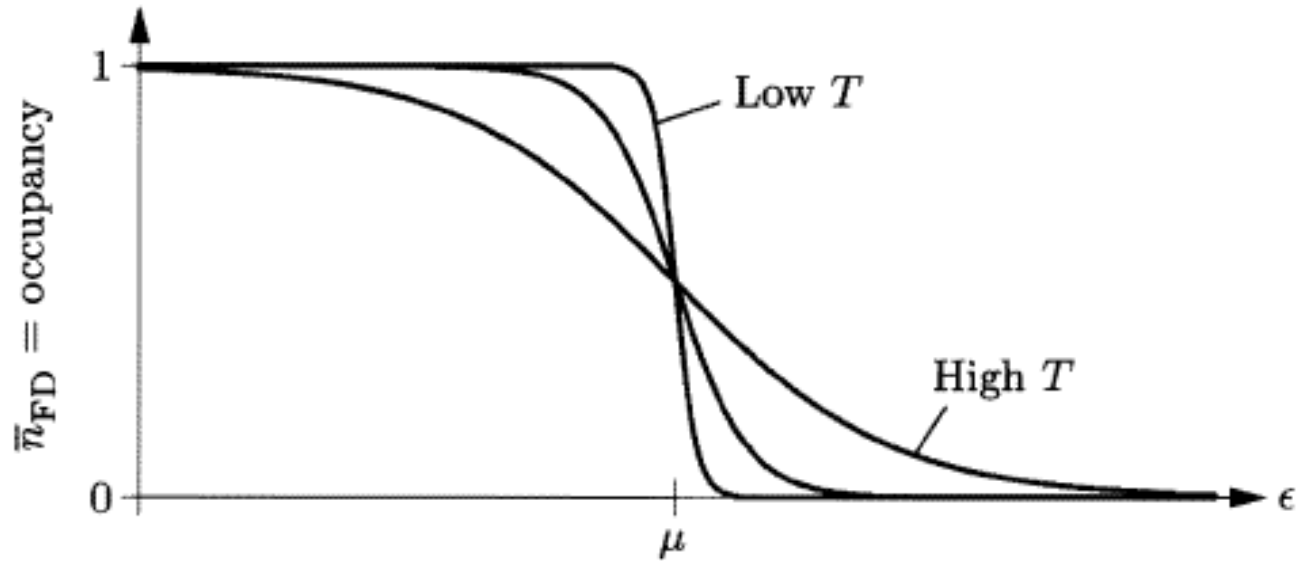
En-partikel tillstånd



$$\mathcal{P}(s) = \frac{1}{\mathcal{Z}} e^{-[E(s) - \mu N(s)]/kT}$$

$$\mathcal{Z} \equiv \sum_s e^{-[E(s) - \mu N(s)]/kT}$$

Fermi-Dirac fördelning



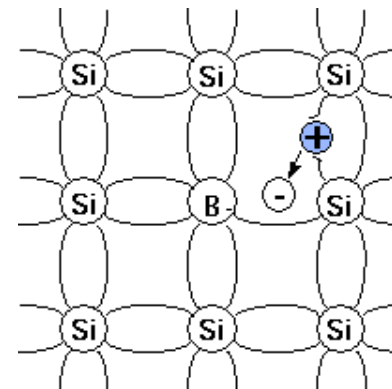
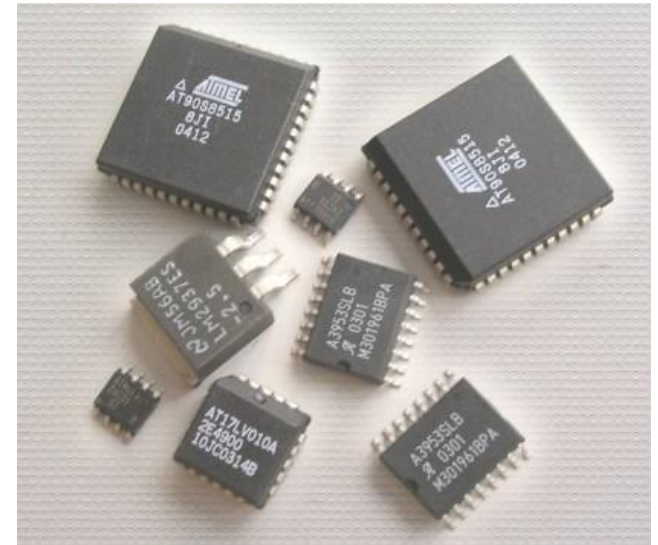
Kan vi förstå egenskaperna för
elektroner i en metall ?



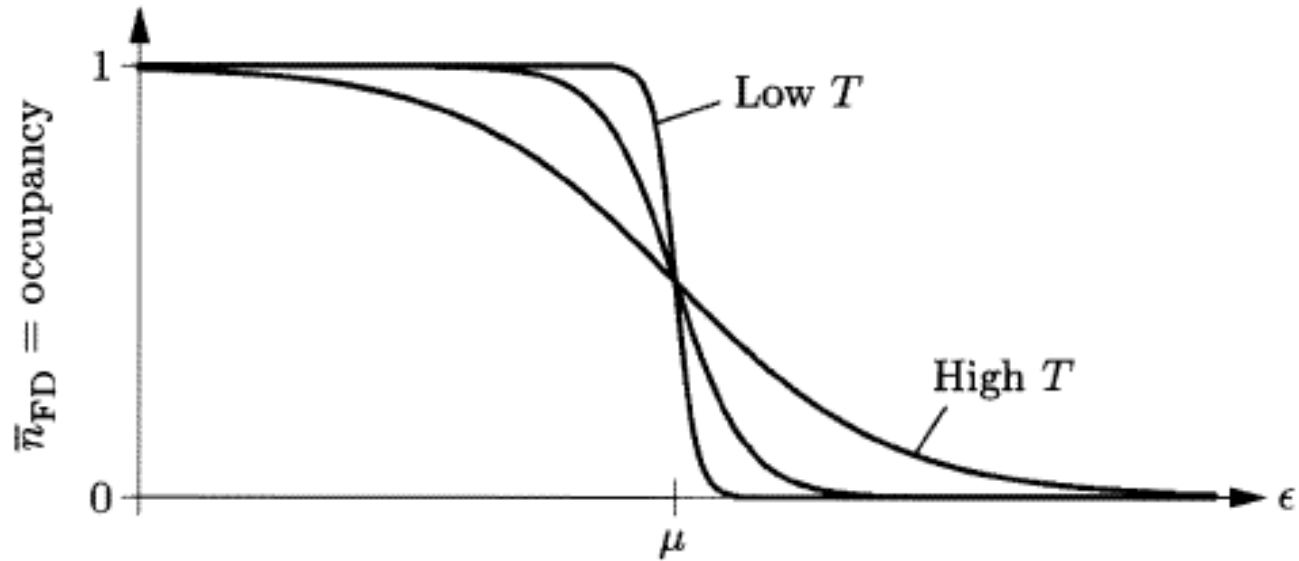
Kan vi förstå stabiliteten av
stjärnor ?



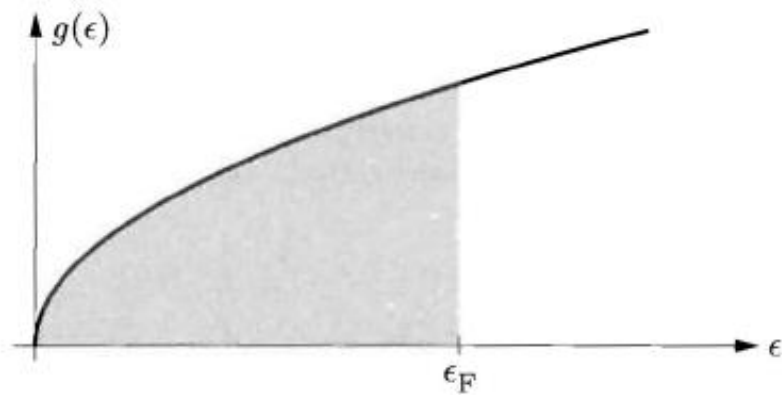
Vad händer när man dopar
halvledare ?



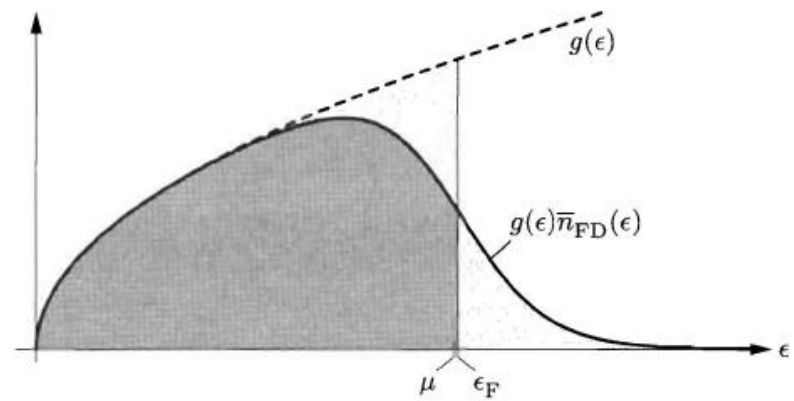
Fermi-Dirac fördelning



Tillståndstätheten



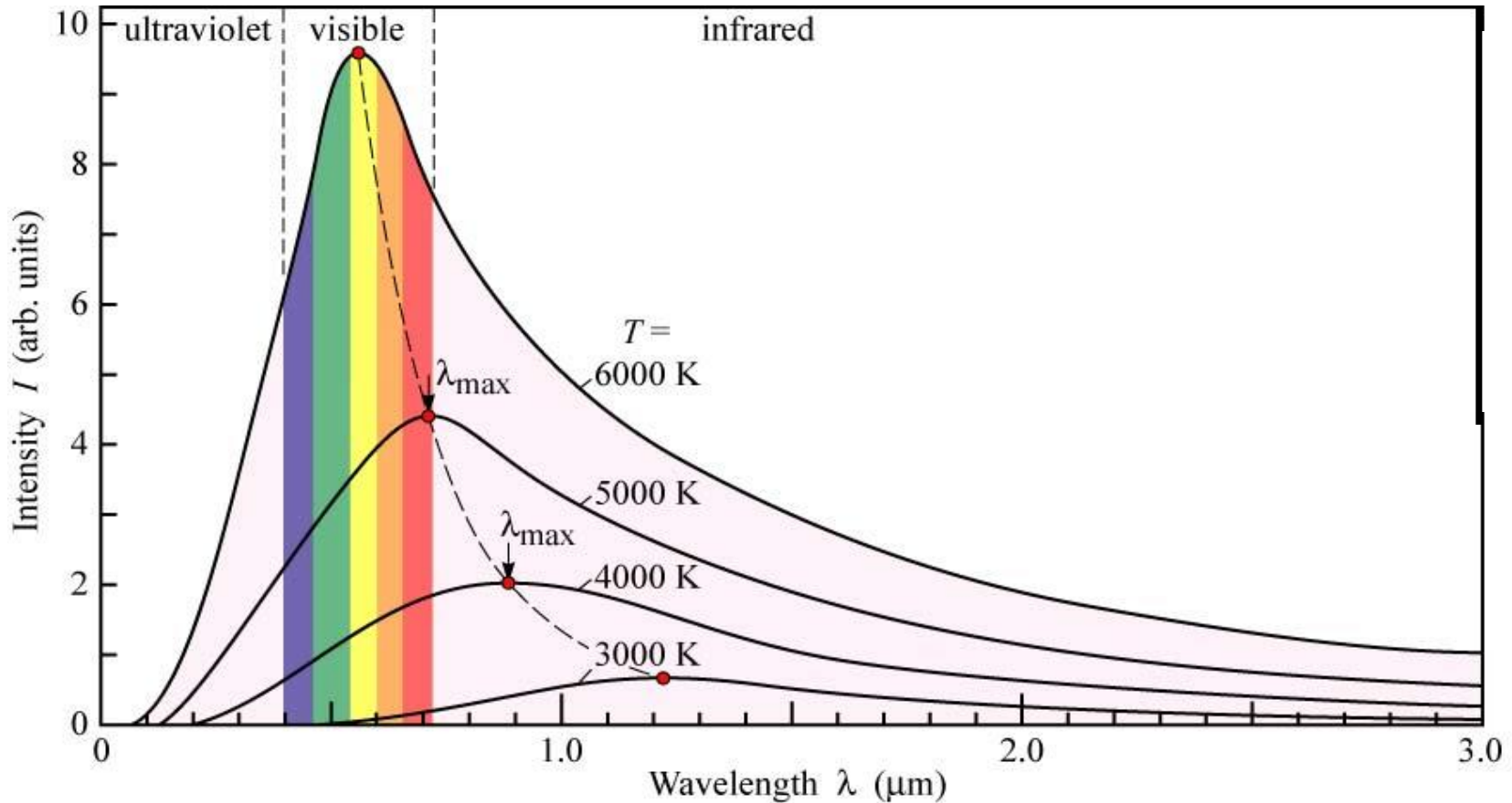
T=0



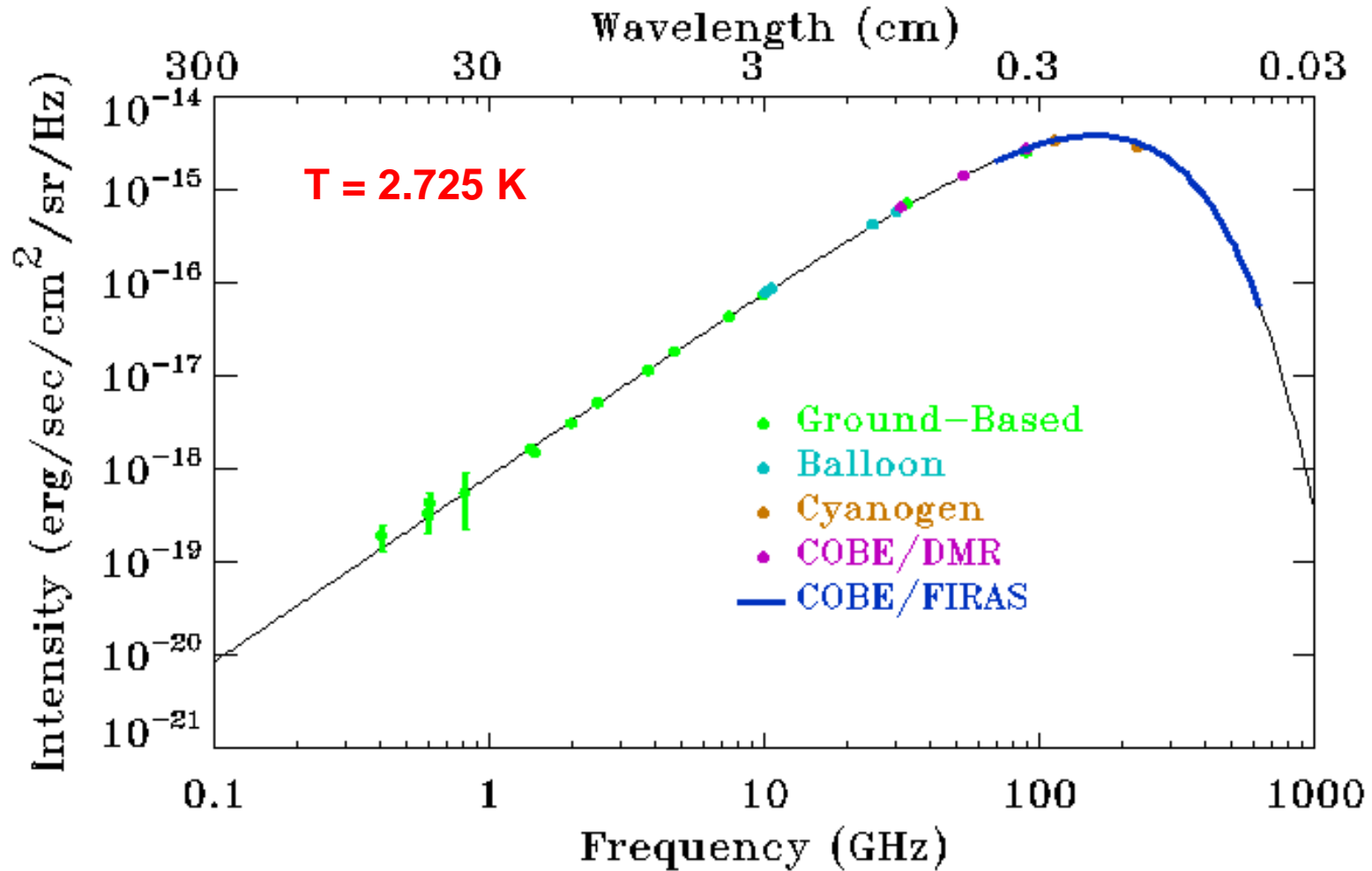
T ändlig men $T \ll T_F$

Fotongas - svartkroppsstrålning

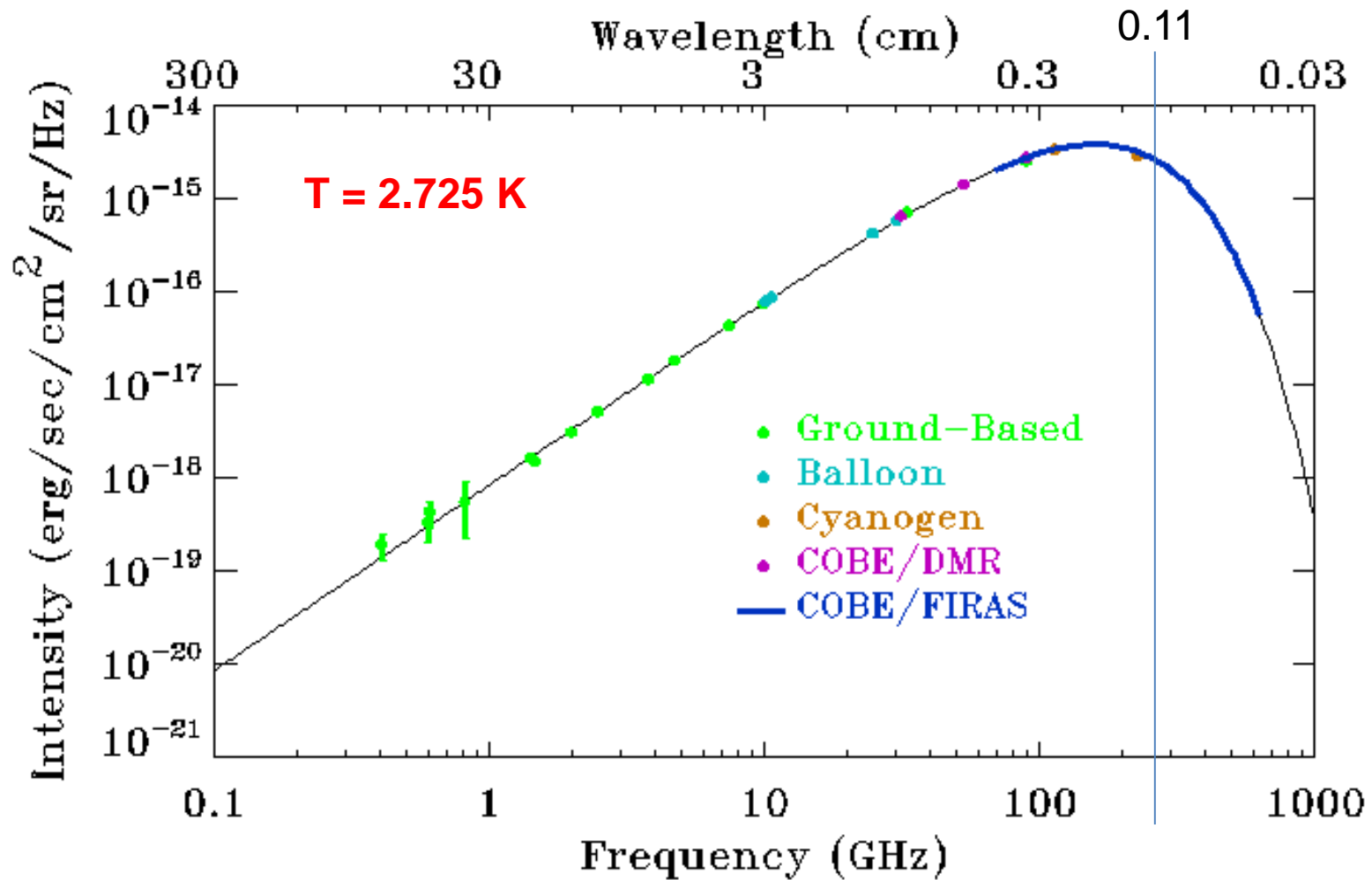
Plancks strålningslag



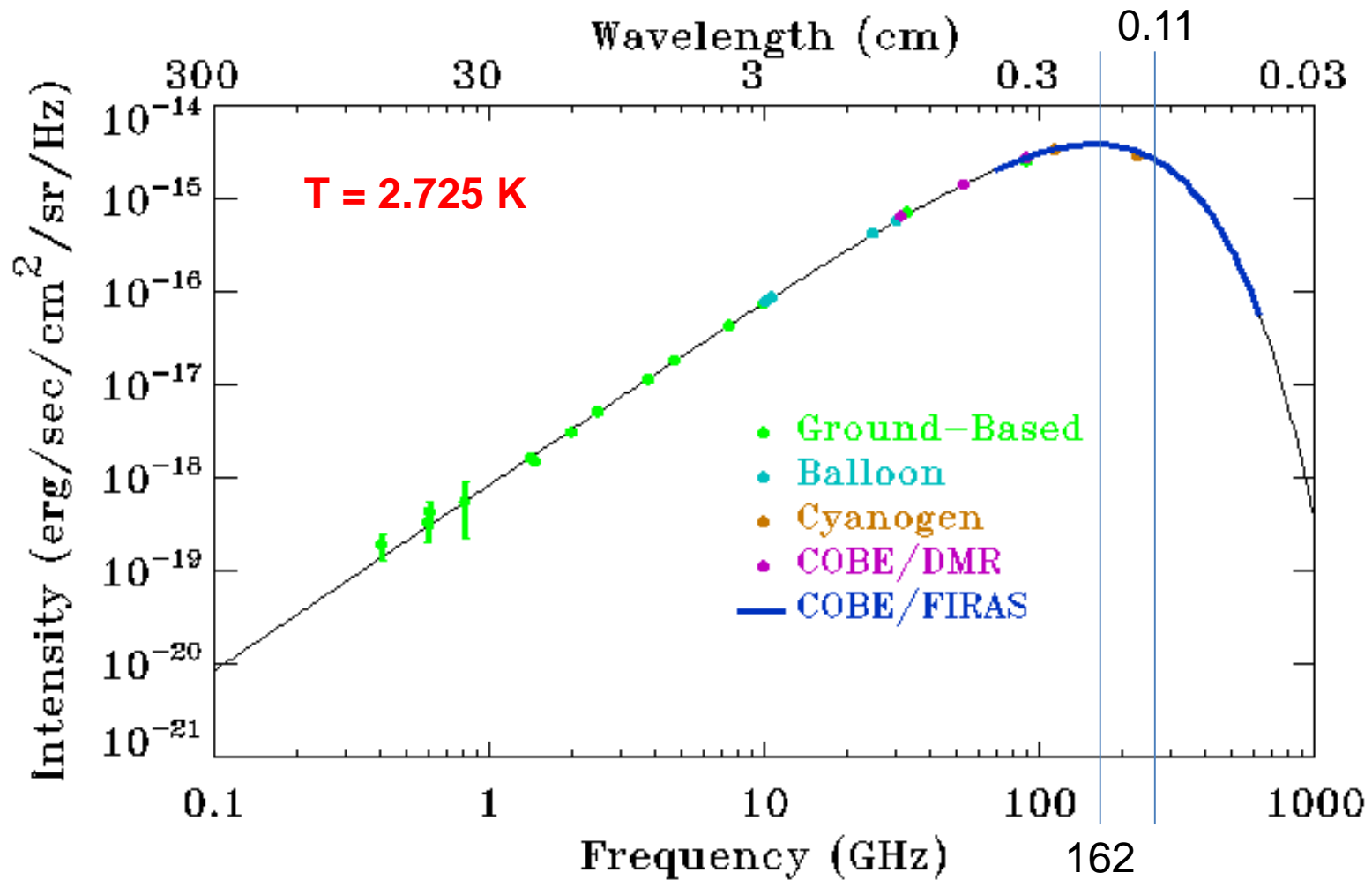
Kosmiska bakgrundsstrålningen



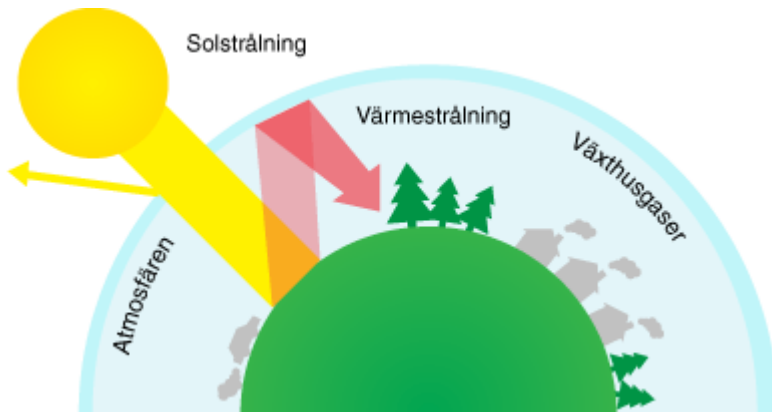
Kosmiska bakgrundsstrålningen



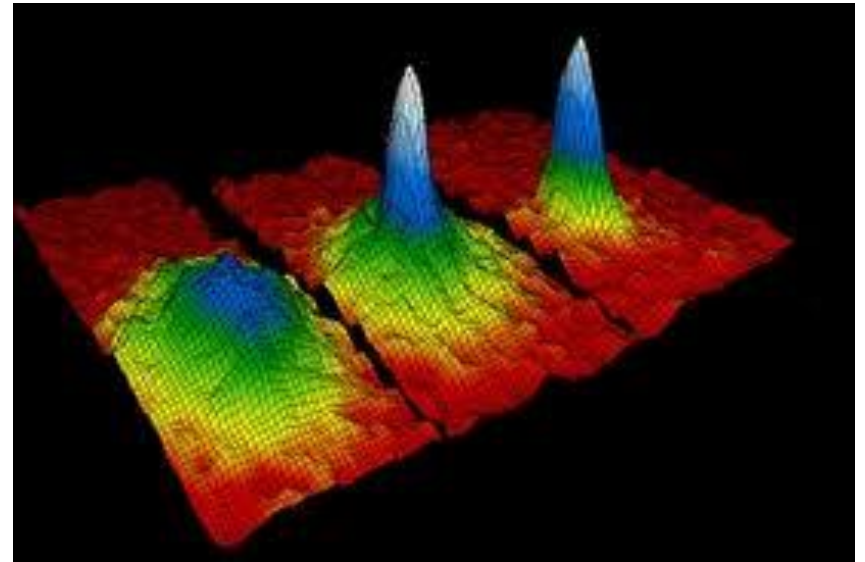
Kosmiska bakgrundsstrålningen



Vad är principen bakom växthuseffekten ?

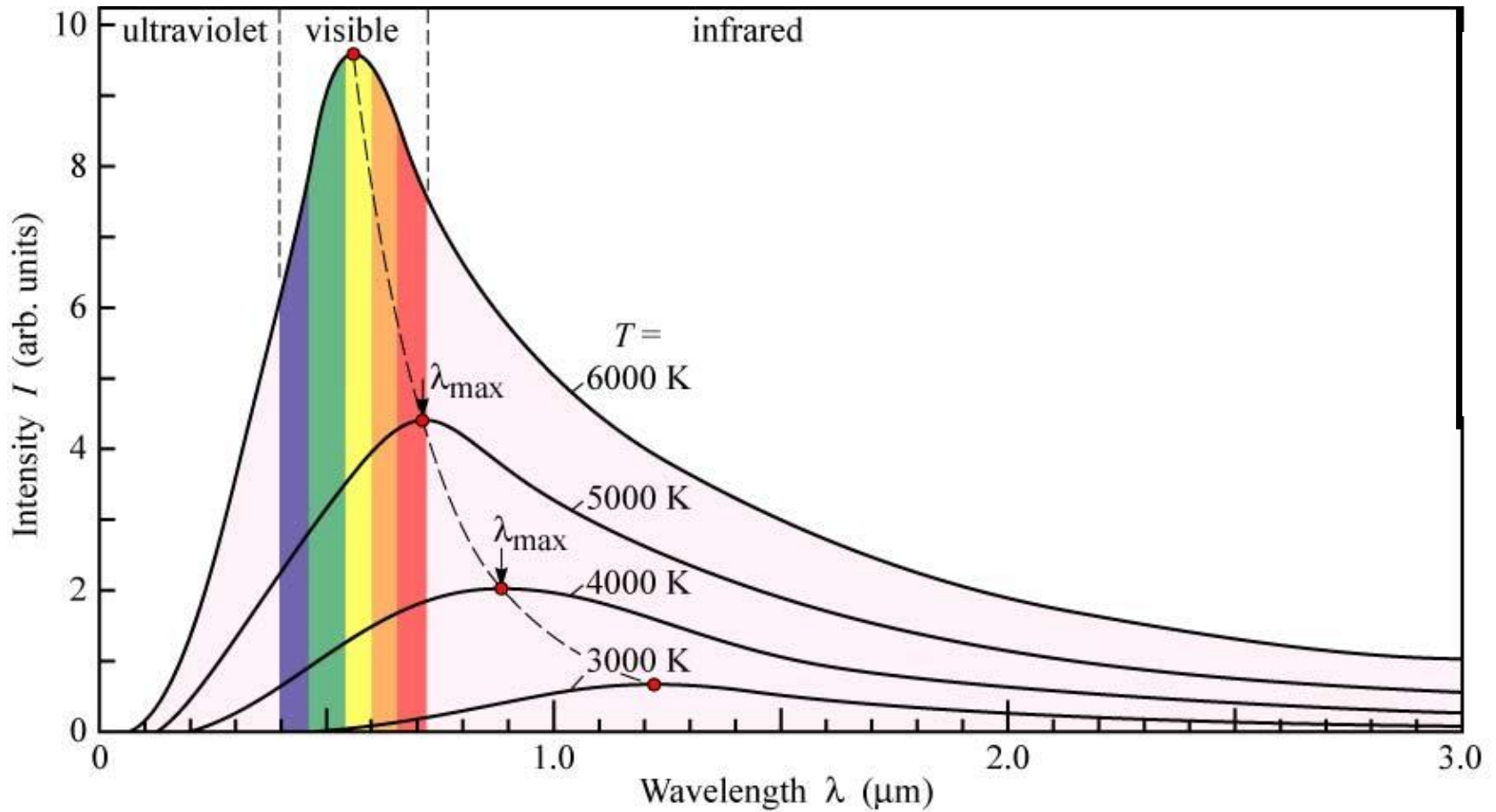


Hur bildas ett koherent kvantkondensat av atomer ?

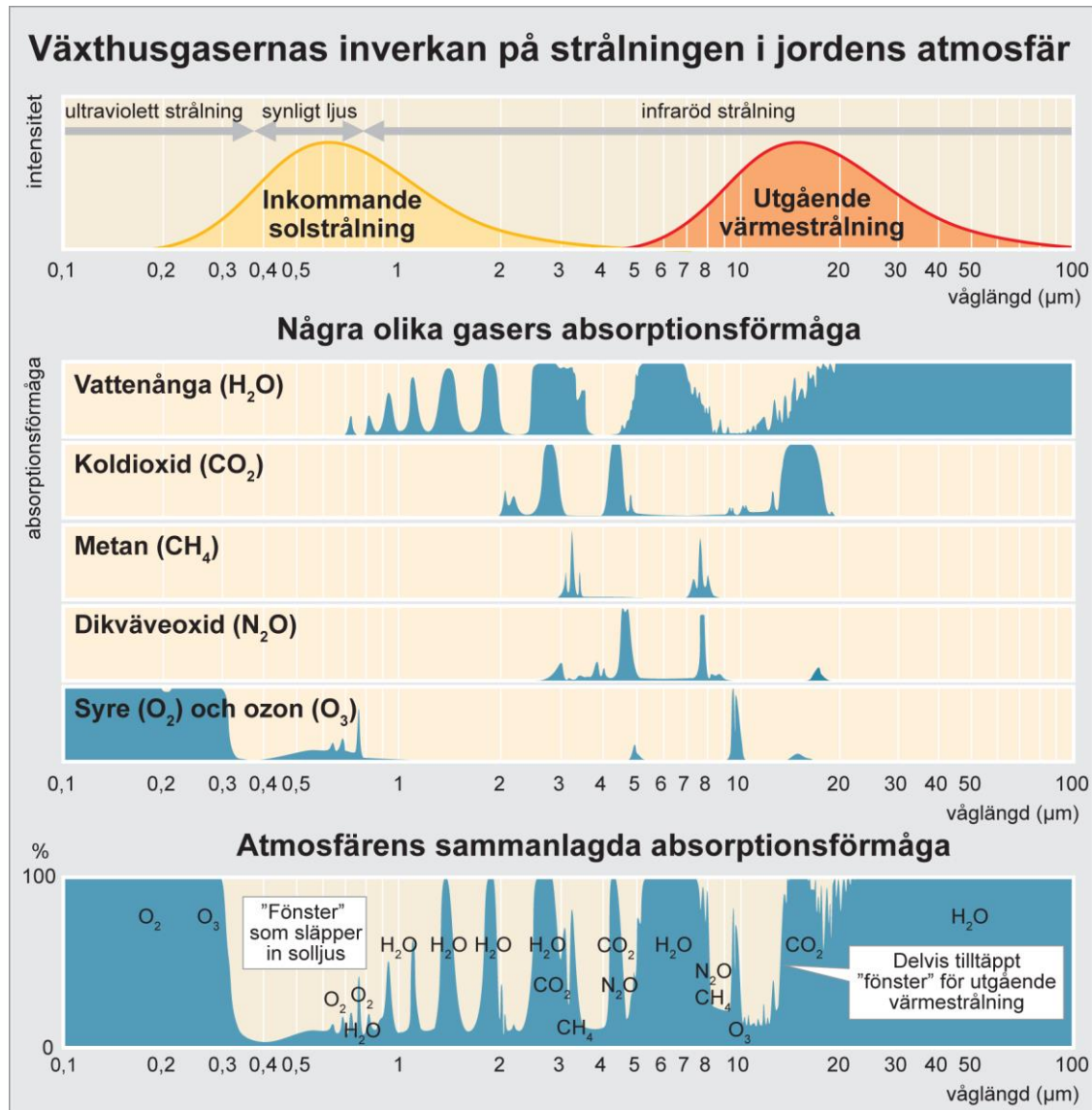


Fotongas - svartkroppsstrålning

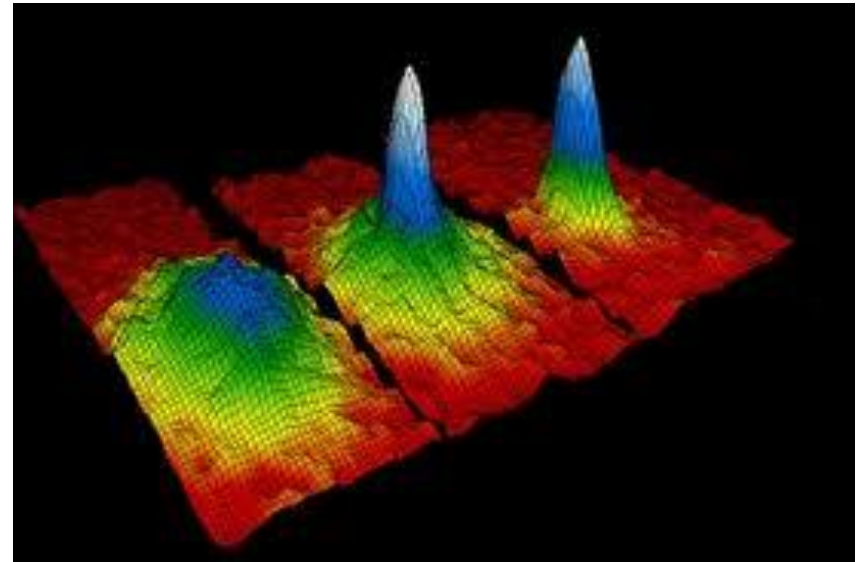
Plancks strålningslag

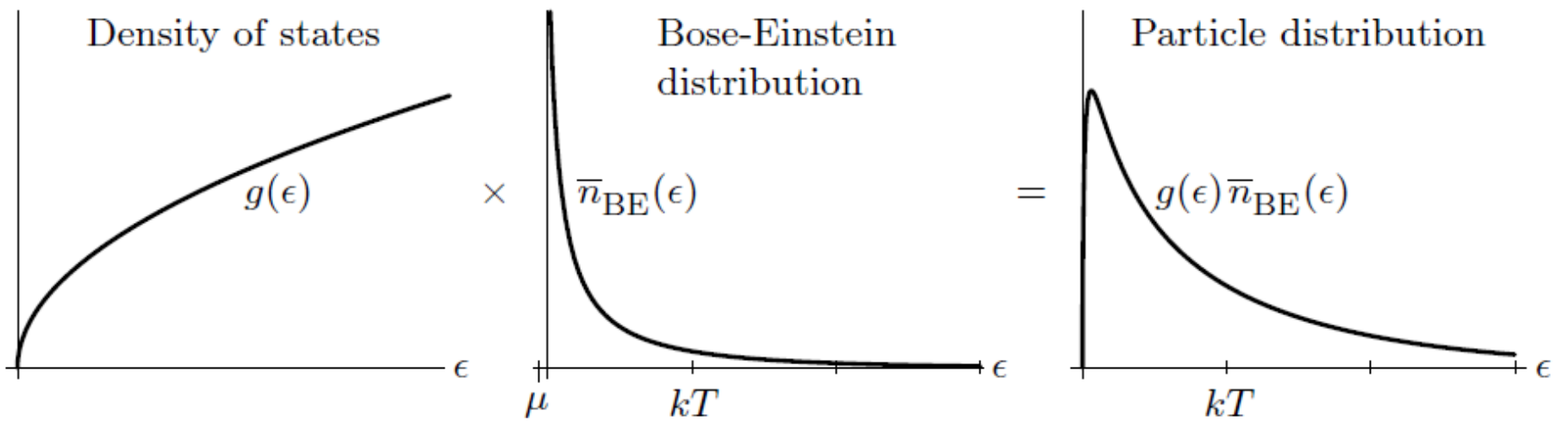


Atmosfärens absorptionsförmåga

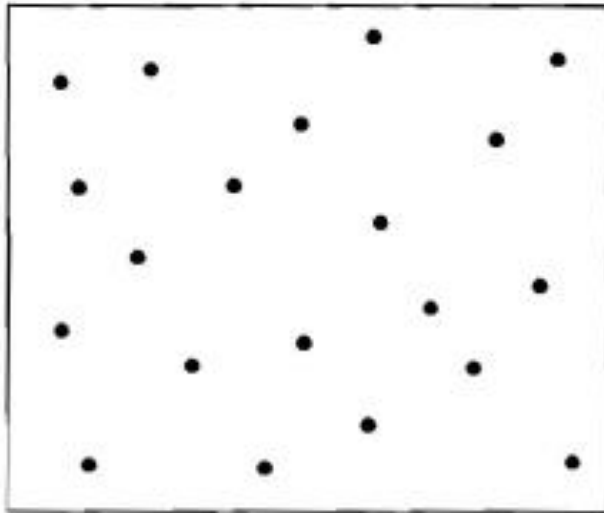


Hur bildas ett koherent
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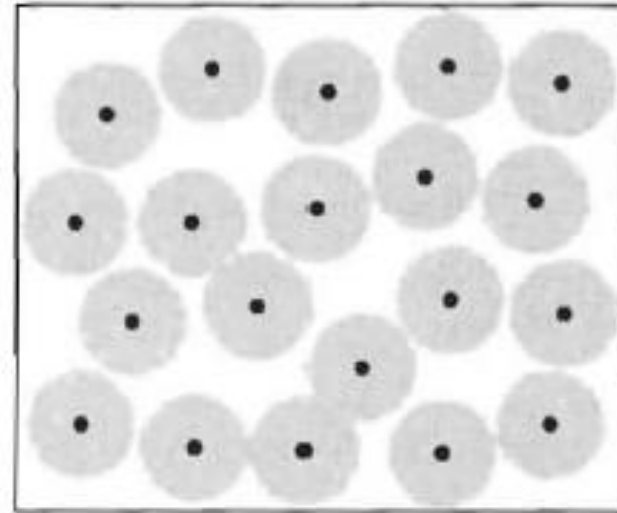




Klassisk \leftrightarrow Kvant-idealgas



Normal gas, $V/N \gg v_Q$



Quantum gas, $V/N \approx v_Q$

Fri partikel i en låda

Klassisk beskrivning

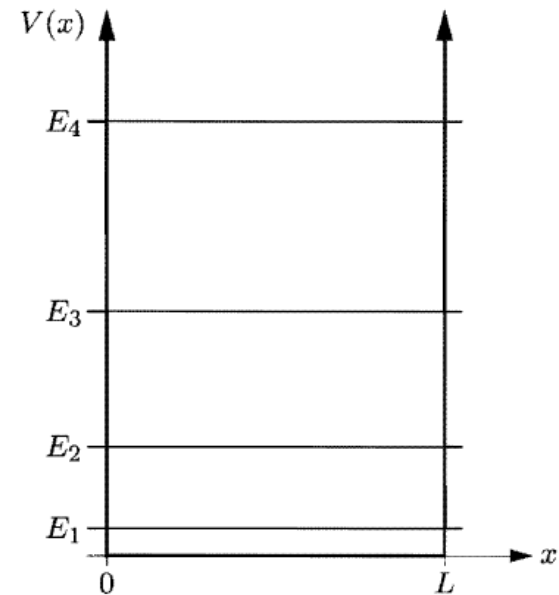
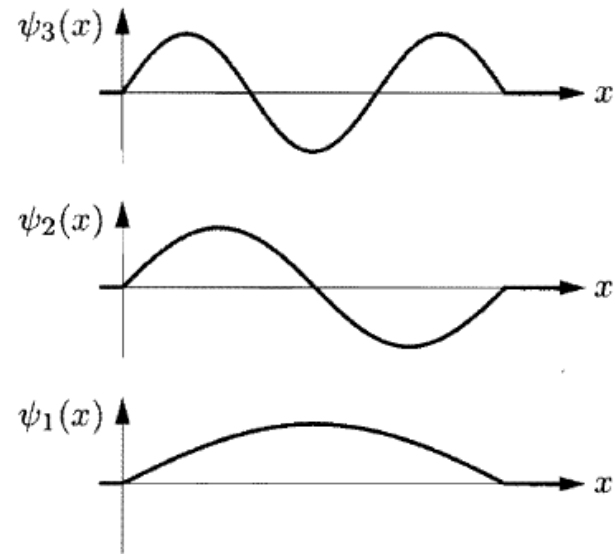
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$$\overline{E_{cl}} = 3 \frac{kT}{2}$$

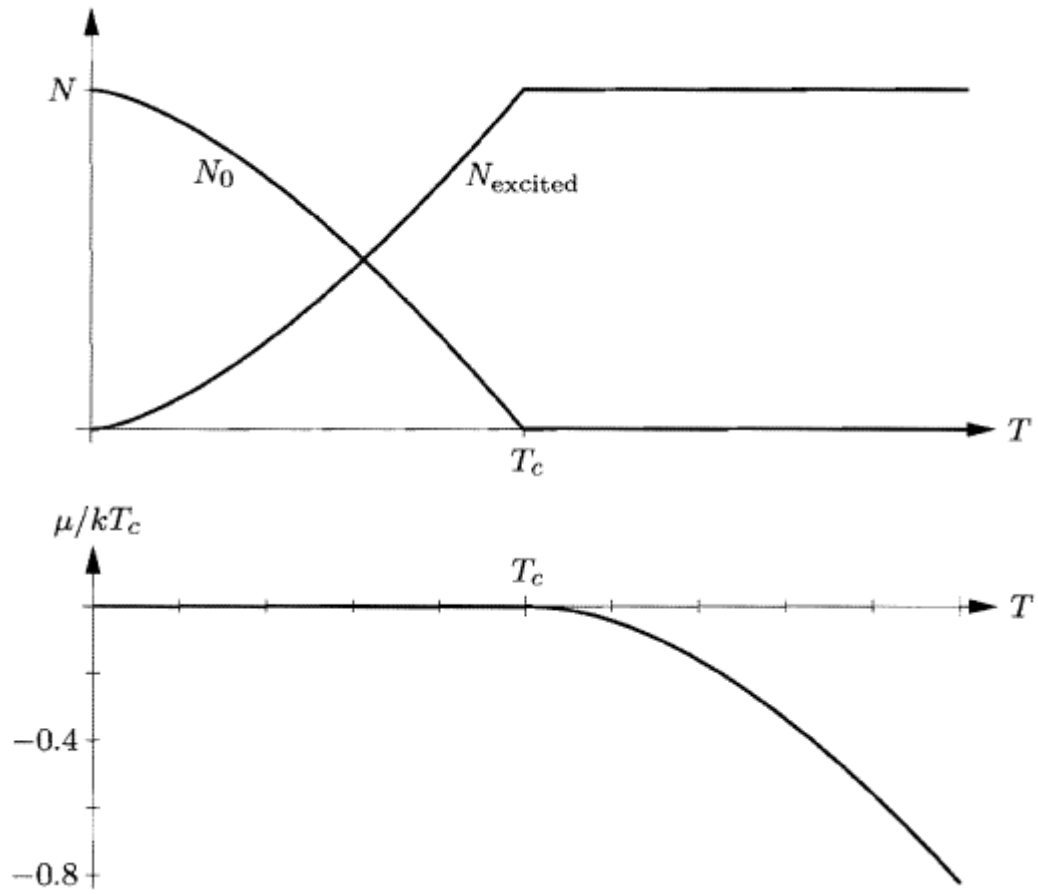
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$$E_{n_x n_y n_z} = \frac{1}{2m} \left(\frac{h}{2L} \right)^2 (n_x^2 + n_y^2 + n_z^2)$$

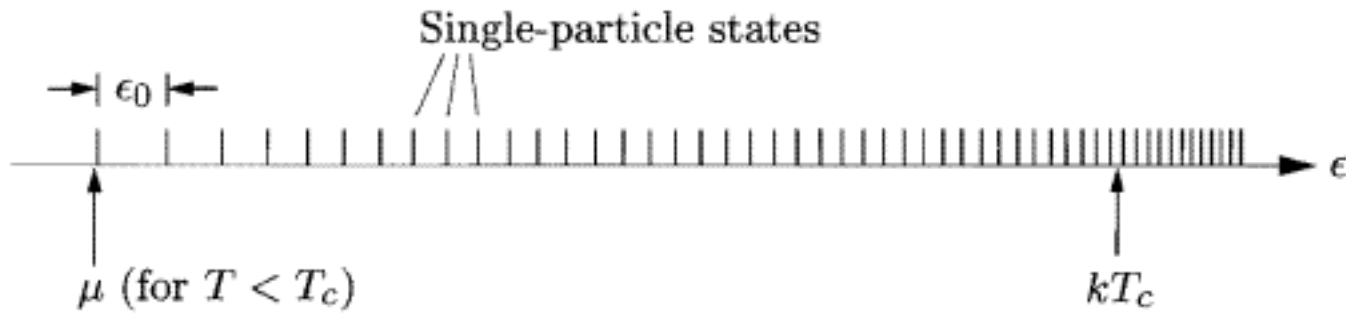
$$n_x, n_y, n_z \in \{1, 2, 3, \dots\}$$



Bose-Einstein kondensation



Kondensations temperaturen T_c



Termodynamik och statistisk mekanik

Termodynamik och statistisk mekanik

- enkla grundläggande antaganden
- kraftfulla metoder
- brett tillämpningsområde

Termodynamikens huvudsatser

Första huvudsatsen

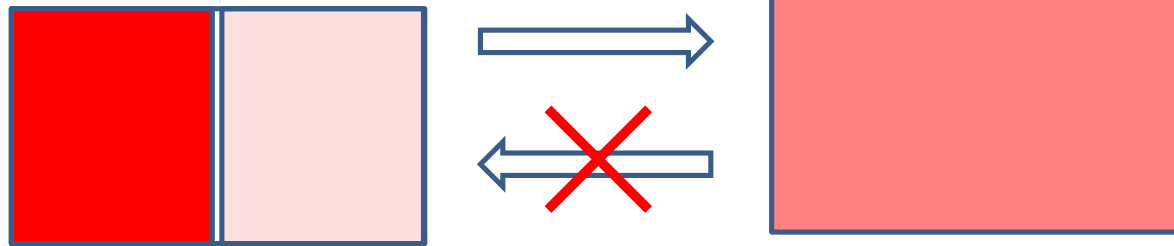
Isolerat system: $\Delta U = 0$

Andra huvudsatsen

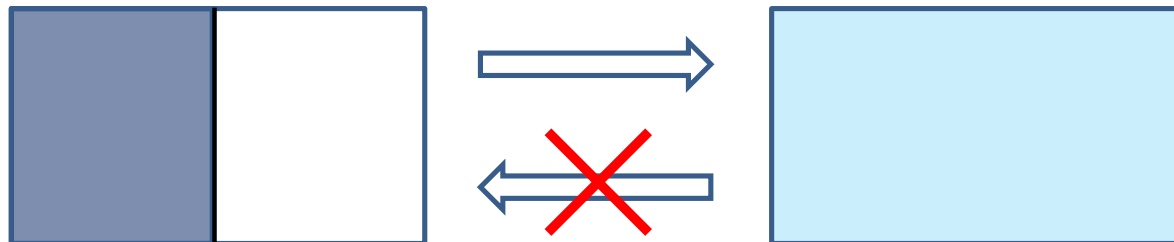
Isolerat system: $\Delta S \geq 0$

Irreversibla processer

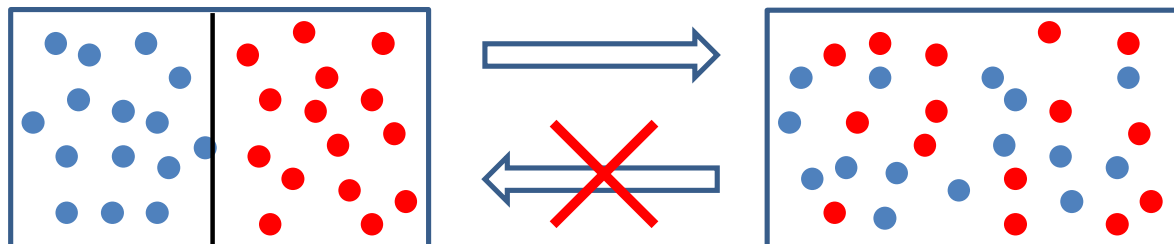
Temperaturutjämnning



Fri expansion



Blandning



Mikrotillstånd

Ett stort antal variabler

i) Kvantmekaniskt

$$\Psi(x_1, \dots, x_F)$$

ii) Klassiskt

$$q_1, \dots, q_F, p_1, \dots, p_F$$

$$F \sim 10^{23}$$

Mekanik

Statistisk



mekanik

Makrotillstånd

Ett fåtal variabler

Termodynamiska tillstånds-
variabler

$$P, V, N, T, U, S, F, G \dots$$

Termodynamik

**Det grundläggande antagandet
i
Statistisk mekanik**

**För ett isolerat system i termisk jämvikt
gäller att
alla tillgängliga mikrotillstånd
är lika sannolika.**

**Det grundläggande antagandet
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You know, the most amazing thing happened to me tonight. I was coming here, on the way to the lecture, and I came in through the parking lot. And you won't believe what happened. I saw a car with the license plate ARW 357! Can you imagine? Of all the millions of license plates in the state, what was the chance that I would see that particular one tonight? Amazing!

—Richard Feynman, quoted by David Goodstein, *Physics Today* **42**, 73 (February, 1989).

ARW 357

You know, the most amazing thing happened to me tonight. I was coming here, on the way to the lecture, and I came in through the parking lot. And you won't believe what happened. I saw a car with the license plate ARW 357! Can you imagine? Of all the millions of license plates in the state, what was the chance that I would see that particular one tonight? Amazing!

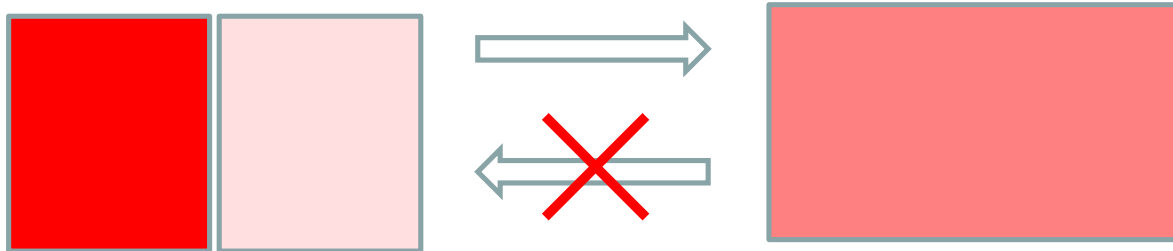
—Richard Feynman, quoted by David Goodstein, *Physics Today* **42**, 73 (February, 1989).

ARW 357

AAA 111

Irreversibla processer

Temperaturutjämning



AAA 111

ARW 357

“It all works because Avogadro’s number is closer to infinity than to 10.”

R. Baierlein

Zentralfriedhof (Central Cemetery) in Vienna, Austria



Boltzmann's definition av entropin

$$S \equiv k \ln \Omega$$

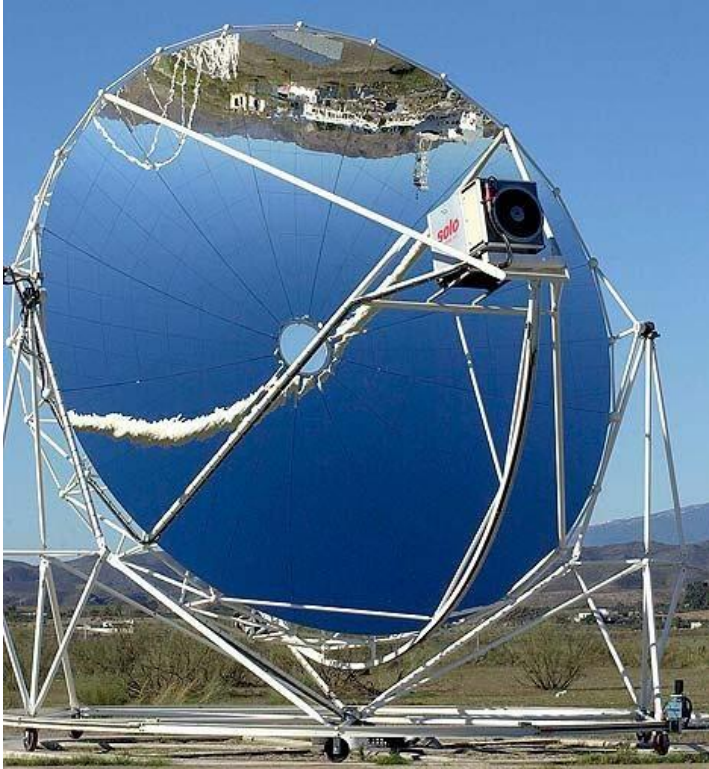
För ett isolerat system gäller att entropin har en tendens att öka

$$\Delta S \geq 0$$

Vid jämvikt kommer systemet befinna sig i det makrotillstånd med maximal entropi (med, för stora system, försumbara fluktuationer).

Termodynamik med tillämpningar

Hur omvandlas värme till elenergi i en Stirlingmotor ?

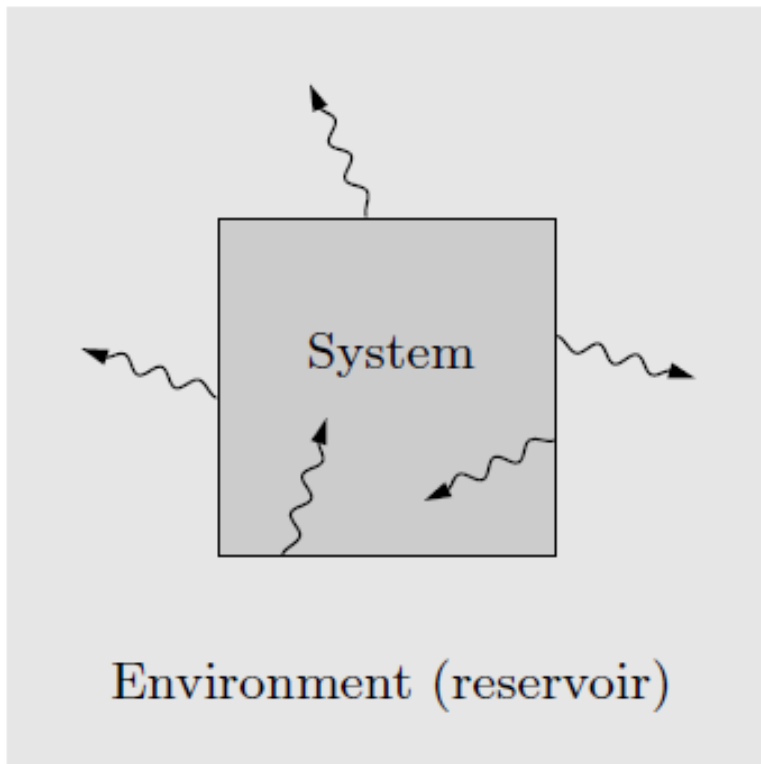


Hur fungerar kompressorkylskåpet ?



Gibbs fria energi

$$G = U + PV - TS$$



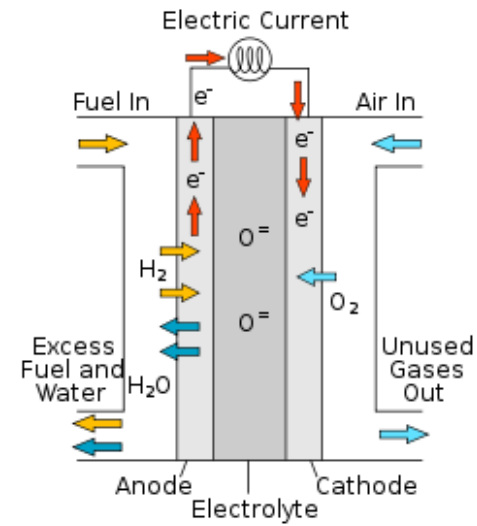
Maximalt arbete

$$W_{\text{ut}} \leq -\Delta G$$

Jämviktsvillkor

G minimum

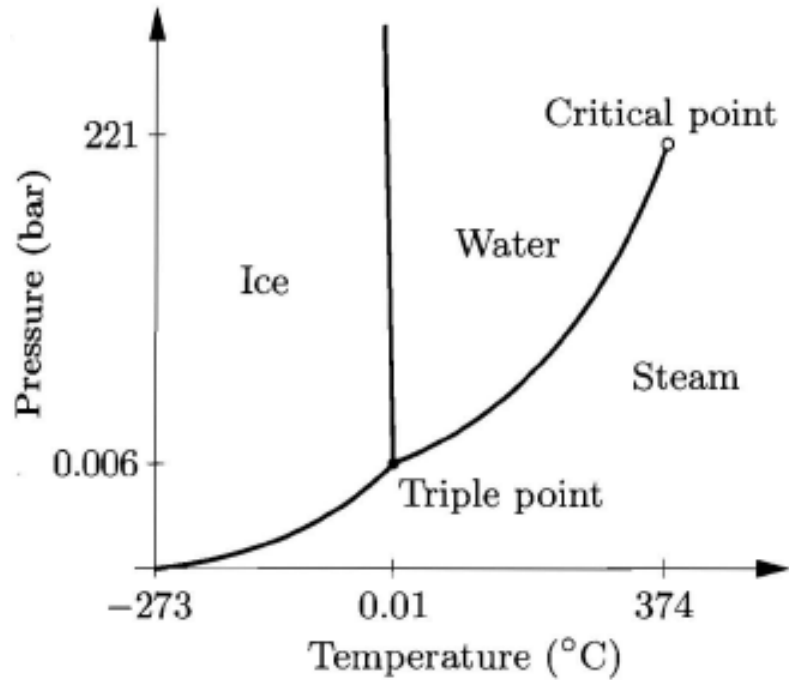
Hur fungerar en bränslecell ?



Smälter isen under skridskon ?



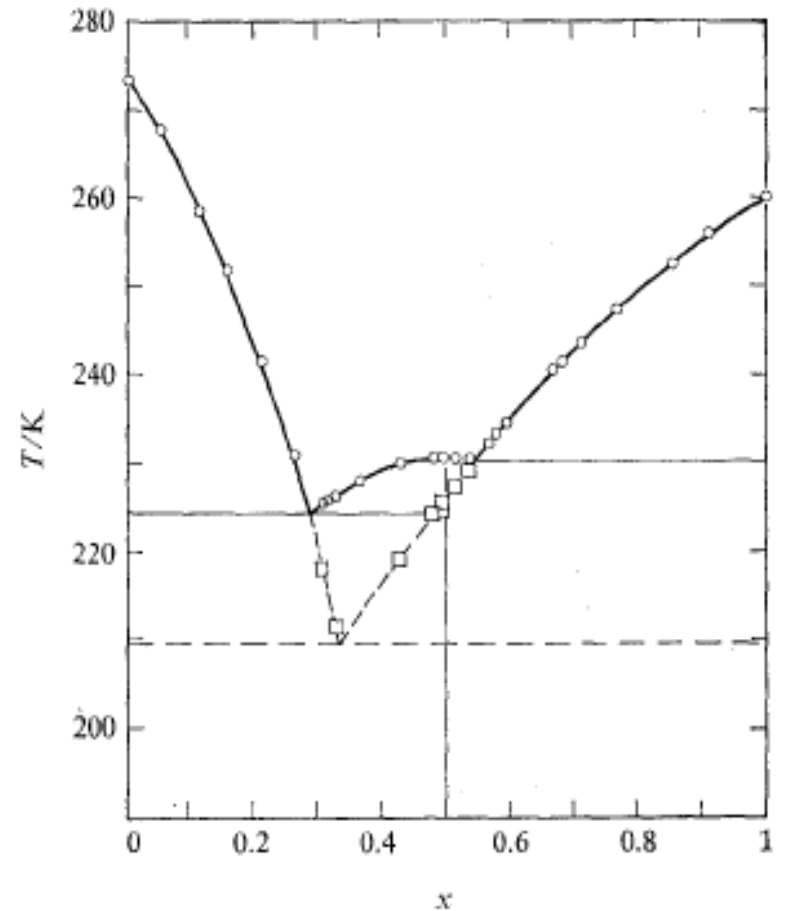
Smälter isen under skridskon ?



När fryser kylarvätskan ?

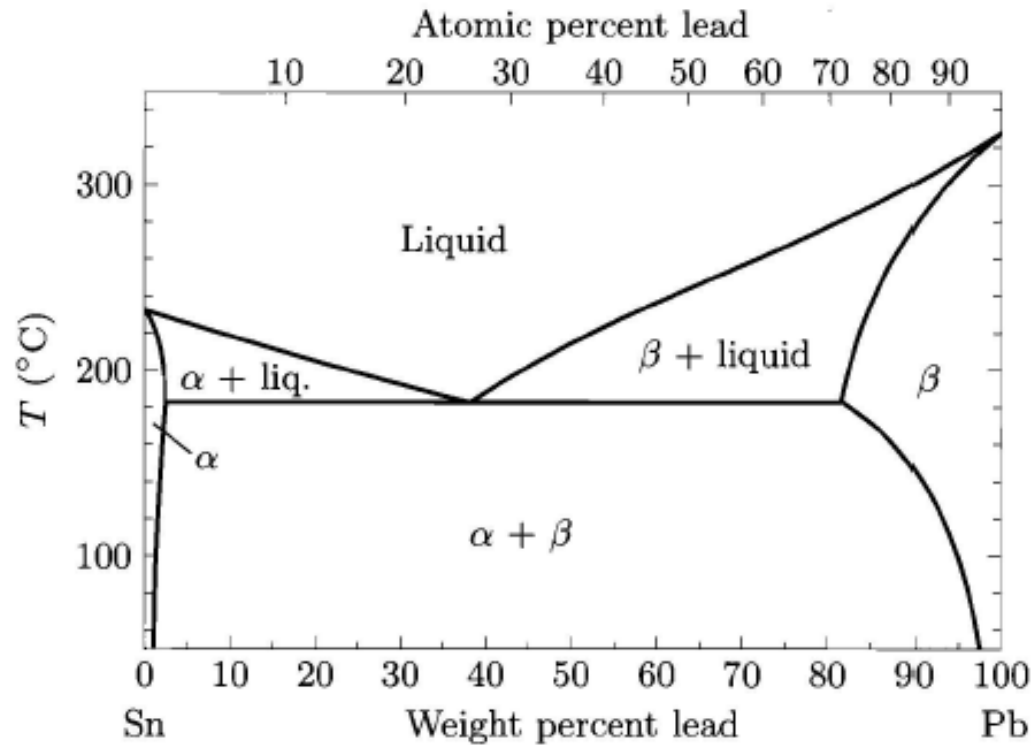


När fryser kylarvätskan ?



J. Bevan Ott, J. Rex Goates, and John D. Lamb,
J. Chem. Thermodynamics 4, 123 (1972).

Eutektiska system



Statistisk mekanik med tillämpningar

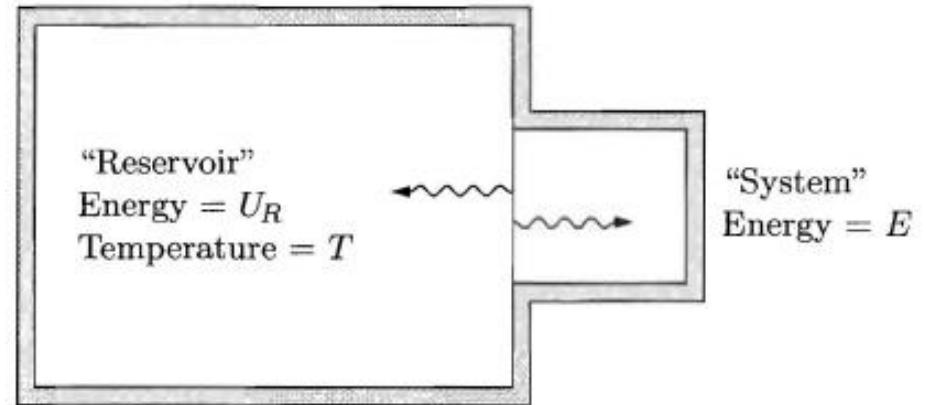
Kanonisk fördelning

Sannolikheten att finna systemet
i mikrotillståndet s

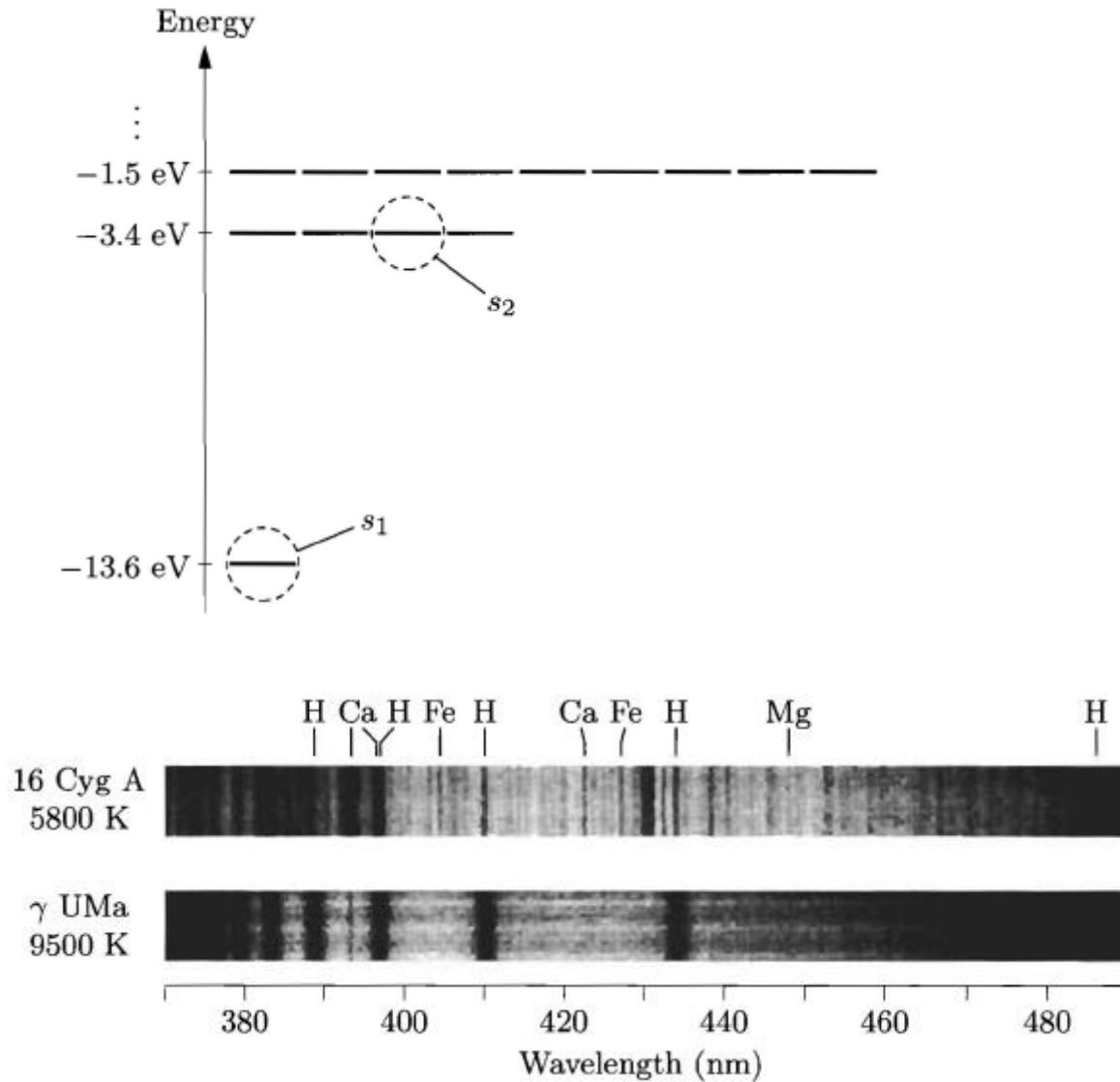
$$\mathcal{P}(s) = \frac{1}{Z} e^{-E(s)/kT}$$

där

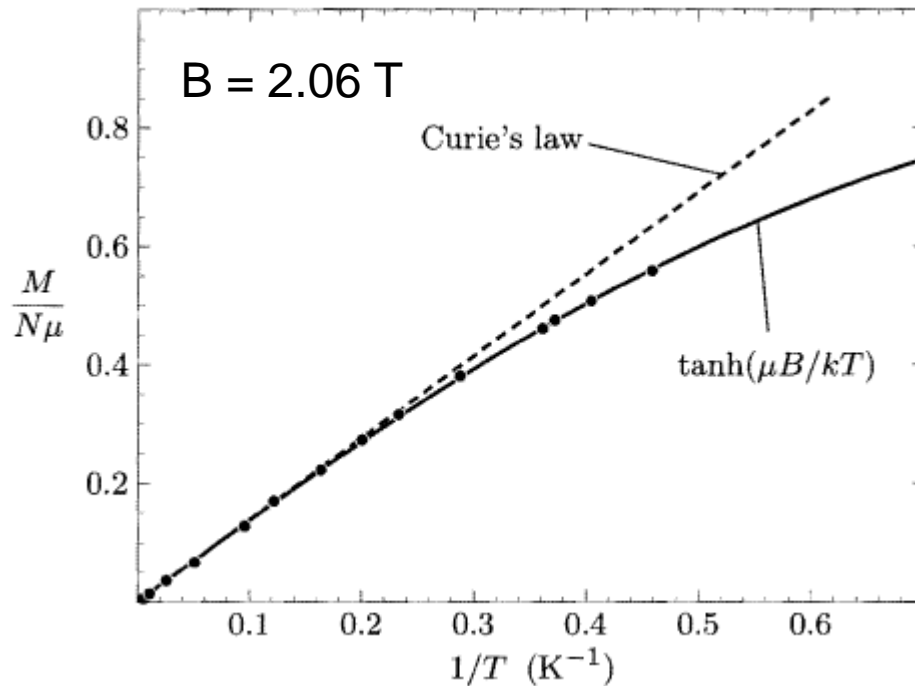
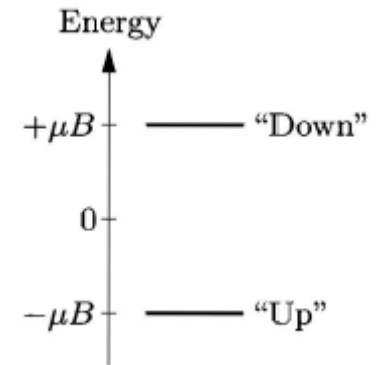
$$Z \equiv \sum_s e^{-E(s)/kT}$$



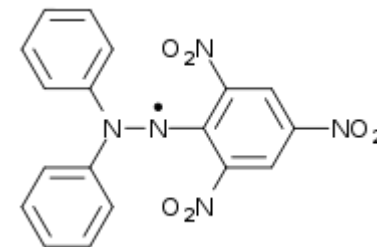
Väteatomen



Paramagnetism

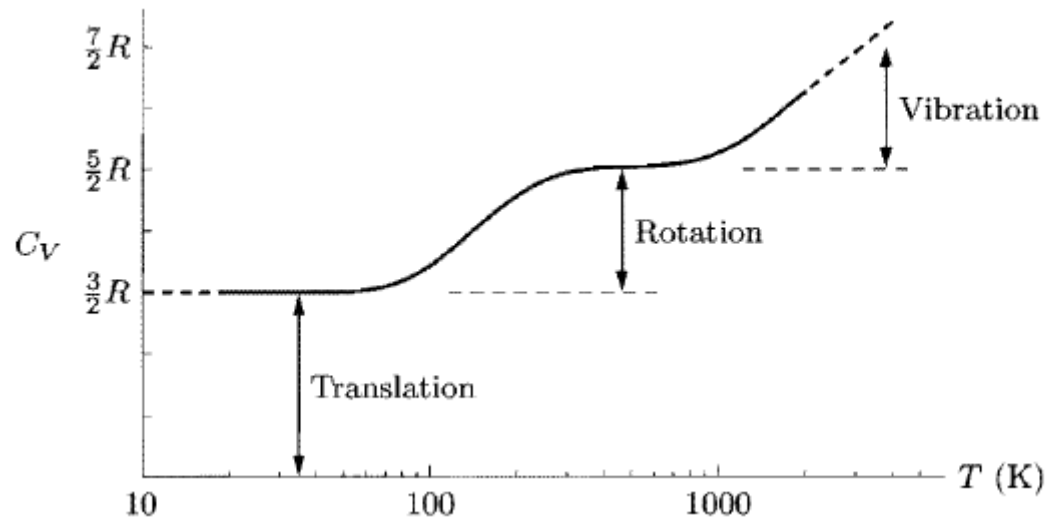


Experimentella data



P. Grobet et al,
J. Chem. Phys. **68**, 5225 (1978)

Gas av molekyler



Fri partikel i en låda

Klassisk beskrivning

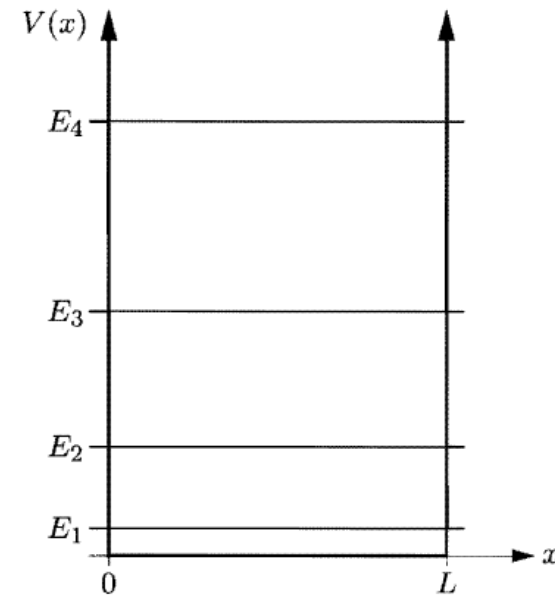
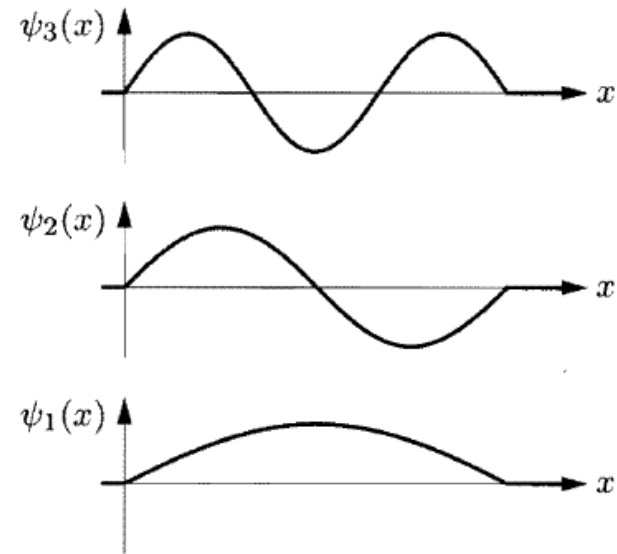
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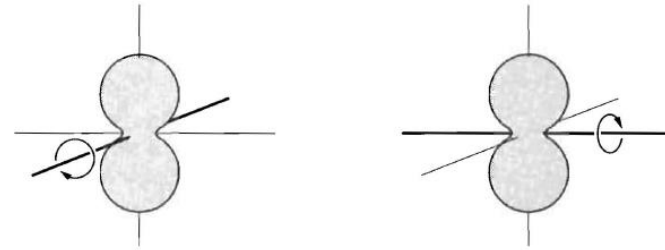


Roterande molekyl

Klassisk beskrivning

$$E_{cl} = \frac{1}{2I}(J_x^2 + J_y^2) ; \quad I = \mu R_0^2$$

$$\overline{E_{cl}} = 2 \frac{kT}{2}$$



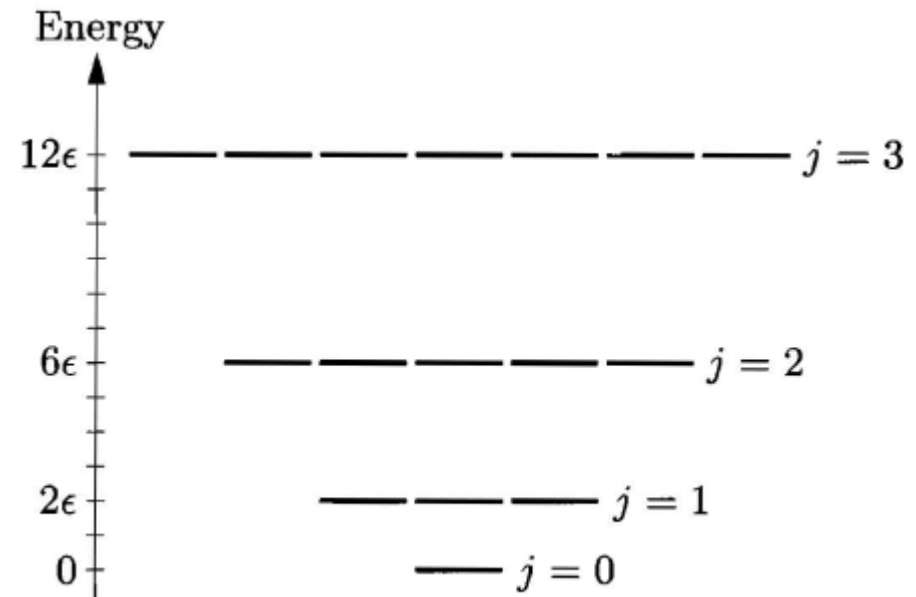
Kvantmekanisk beskrivning

$$E_j = \frac{\hbar^2}{2I}j(j+1) , \quad g_j = 2j+1$$

$$j = 0, 1, 2, \dots$$

Typisk energiuppsplittring

$$k\theta_{rot} \equiv \frac{\hbar^2}{2I}$$



Vibrerande molekyl

Klassisk beskrivning

$$E_{cl} = \frac{p^2}{2\mu} + \frac{k_s}{2}q^2 ; \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$\overline{E_{cl}} = 2 \frac{kT}{2}$$

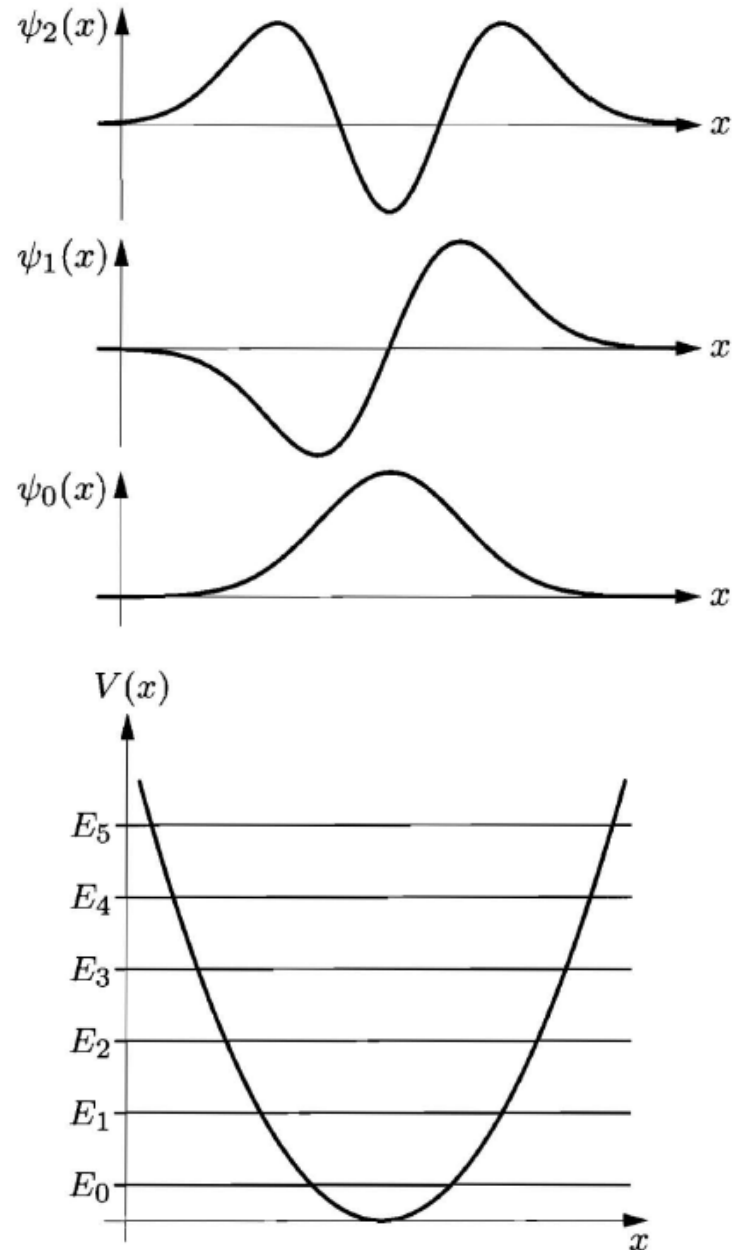
Kvantmekanisk beskrivning

$$E_n = \left(n + \frac{1}{2}\right)hf ; \quad f = \frac{1}{2\pi} \sqrt{\frac{k_s}{\mu}}$$

$$n = 0, 1, 2, \dots$$

Typisk energiuppsplittring

$$k\theta_{vib} \equiv hf$$



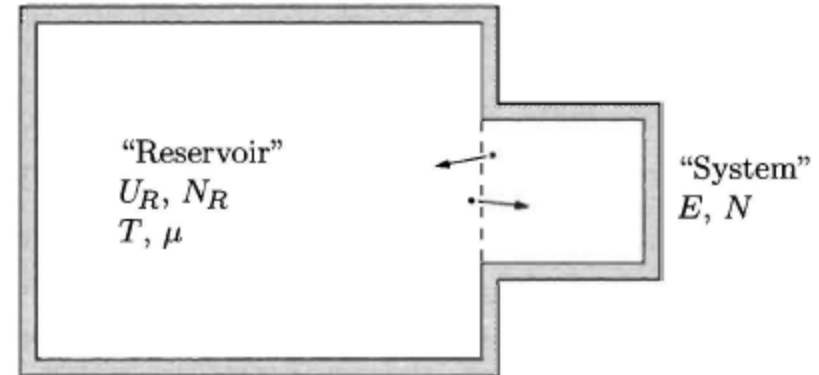
Stor kanonisk fördelning

Sannolikheten att finna systemet i mikrotillståndet s

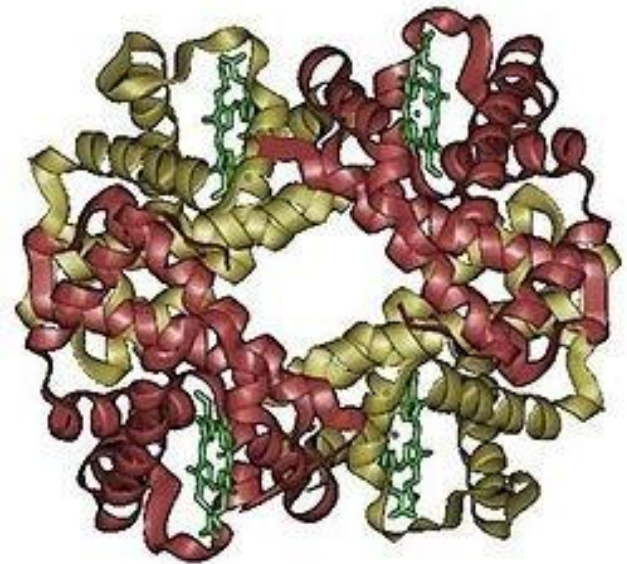
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där

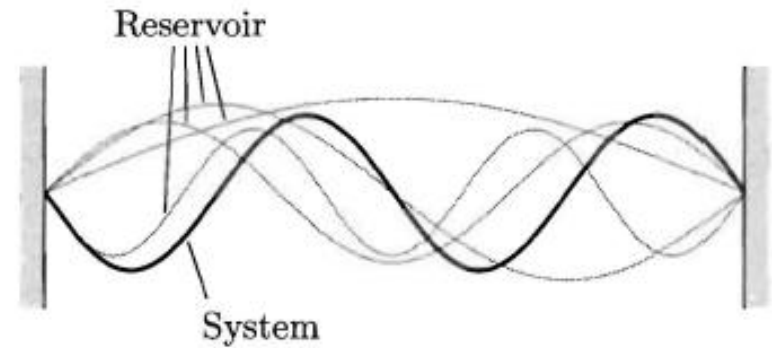
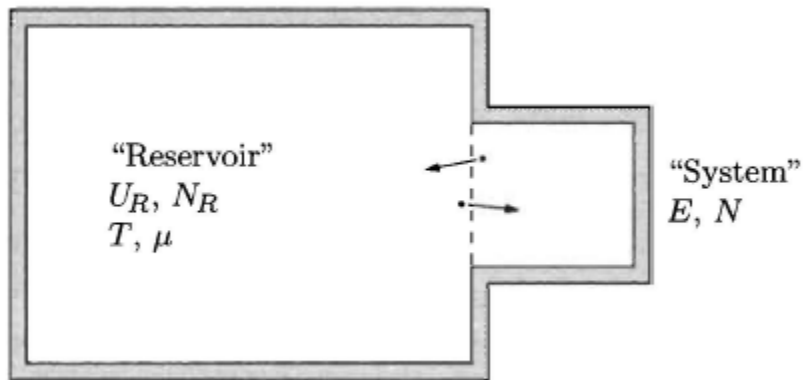
$$\mathcal{Z} \equiv \sum_s e^{-[E(s) - \mu N(s)]/kT}$$



Hur blir man koloxidförgiftad ?



En-partikel tillstånd



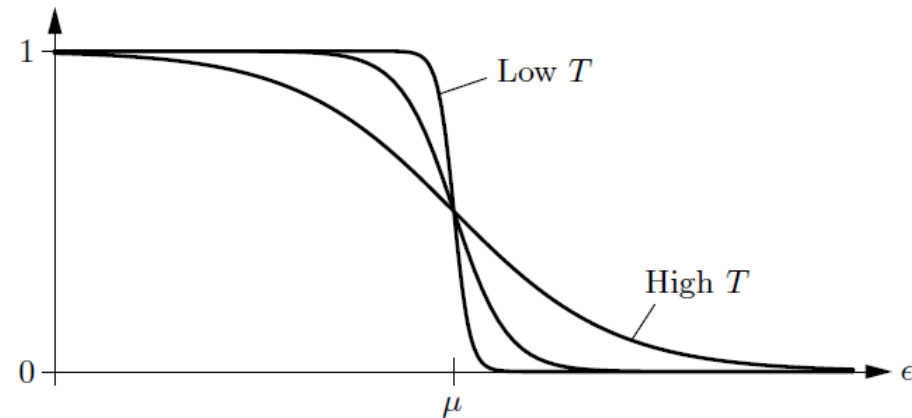
Kan vi förstå egenskaperna för
elektroner i en metall ?



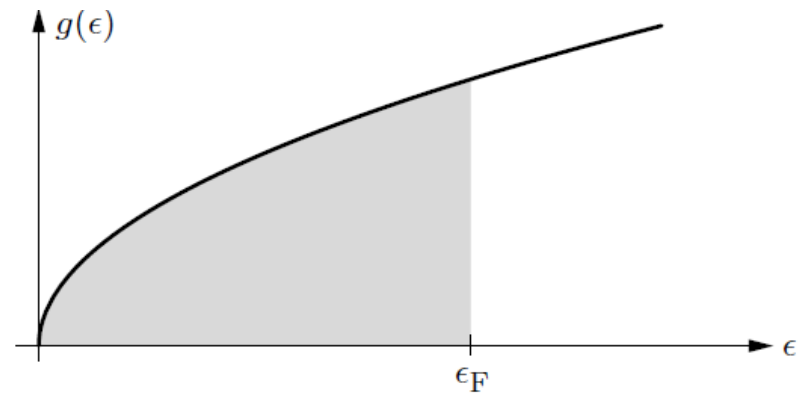
Kan vi förstå egenskaperna för elektroner i en metall ?



Fördelningsfunktion



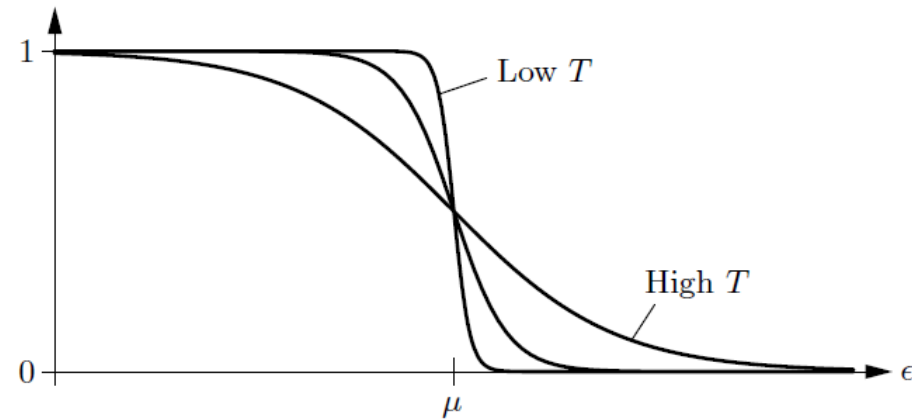
Tillståndstäthet



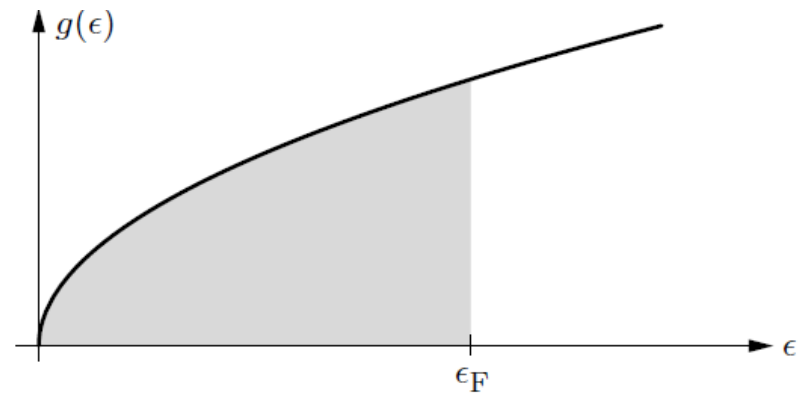
Kan vi förstå stabiliteten av
stjärnor ?



Fördelningsfunktion



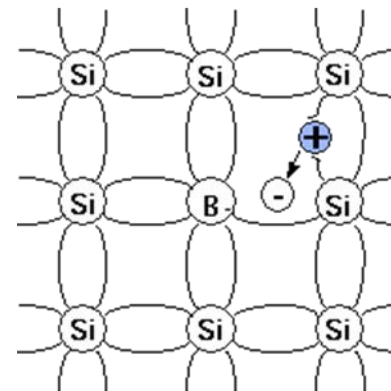
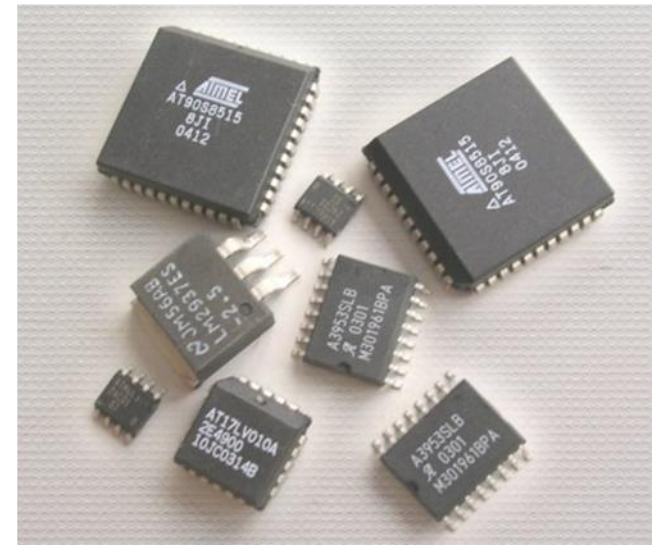
Tillståndstäthet



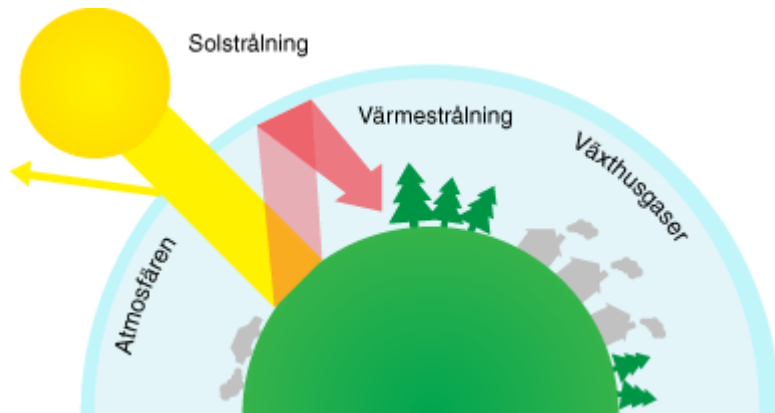
Kan vi förstå egenskaperna för elektroner i en metall ?



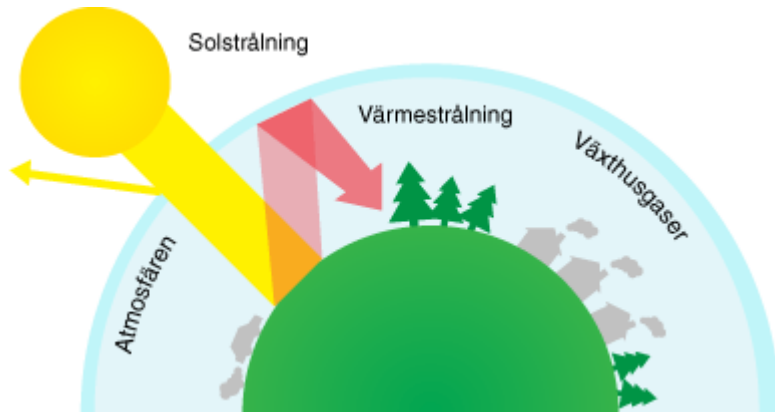
Vad händer när man dopar halvledare ?



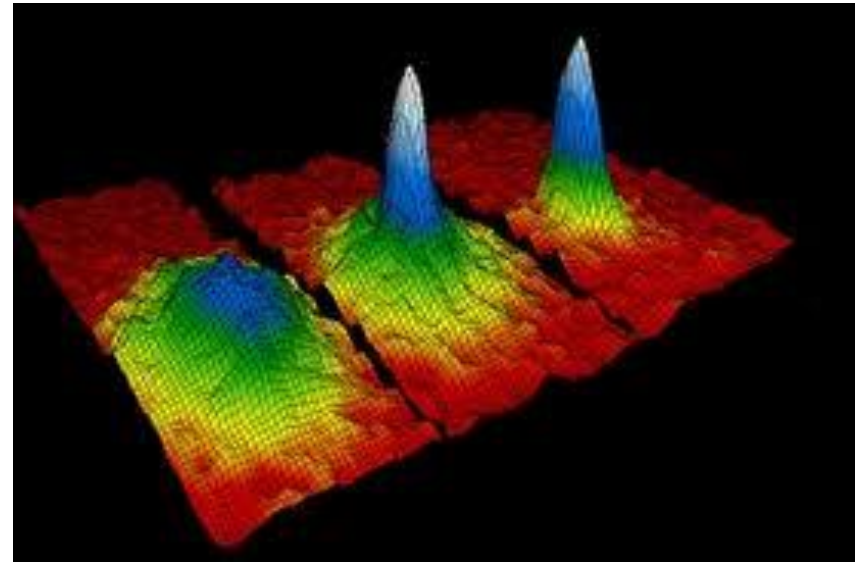
Vad är principen bakom
växthuseffekten ?



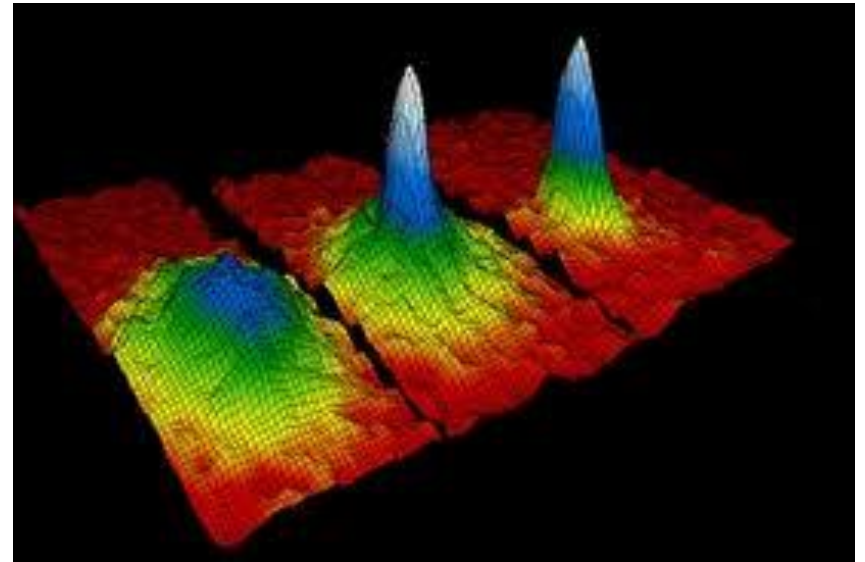
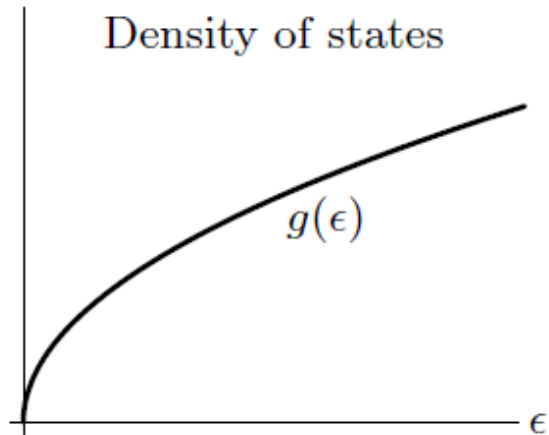
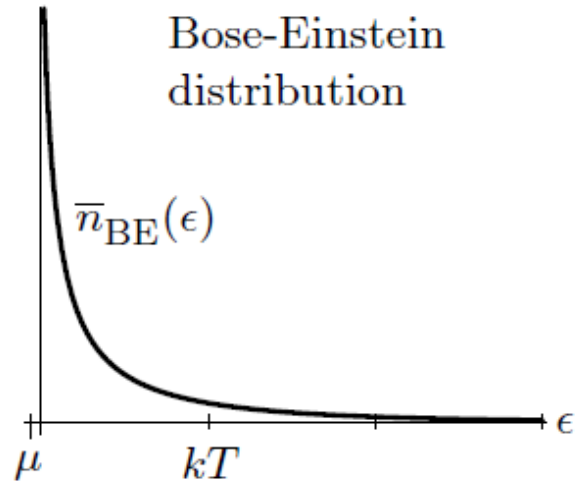
Vad är principen bakom växthuseffekten ?



Hur bildas ett koherent kvantkondensat av atomer ?



Hur bildas ett koherent kvantkondensat av atomer ?



Välkomna till kursen i

Termodynamik och statistisk mekanik

Termodynamik och statistisk mekanik

- enkla grundläggande antaganden
- kraftfulla metoder
- brett tillämpningsområde

Avogadro's number: $N_A = 6.02 \cdot 10^{23}$

“It all works because Avogadro's number is closer to infinity than to 10.”

R. Baierlein

Mikrotillstånd

Ett stort antal variabler

i) Kvantmekaniskt

$$\Psi(x_1, \dots, x_F)$$

ii) Klassiskt

$$q_1, \dots, q_F, p_1, \dots, p_F$$

$$F \sim 10^{23}$$

Mekanik

Statistisk



mekanik

Makrotillstånd

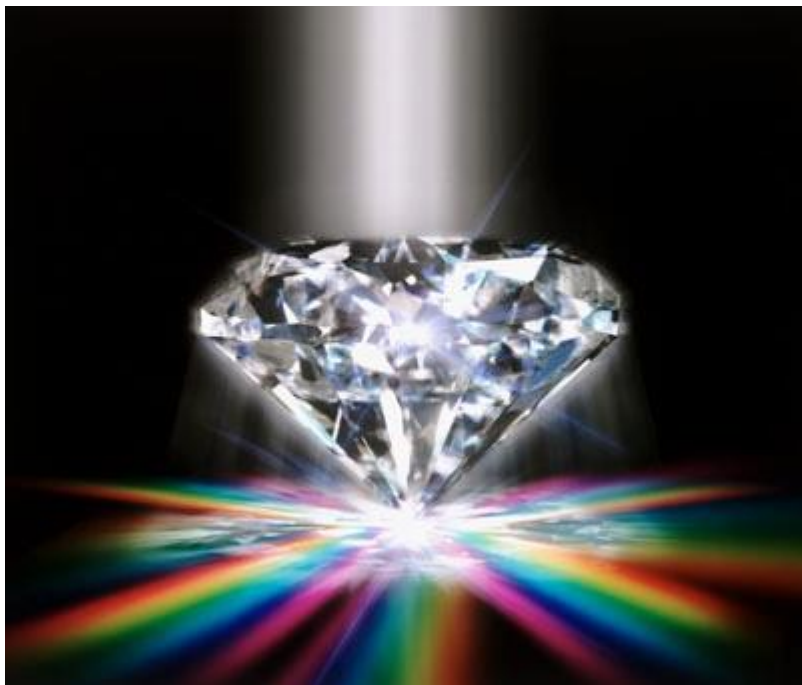
Ett fåtal variabler

Termodynamiska tillstånds-
variabler

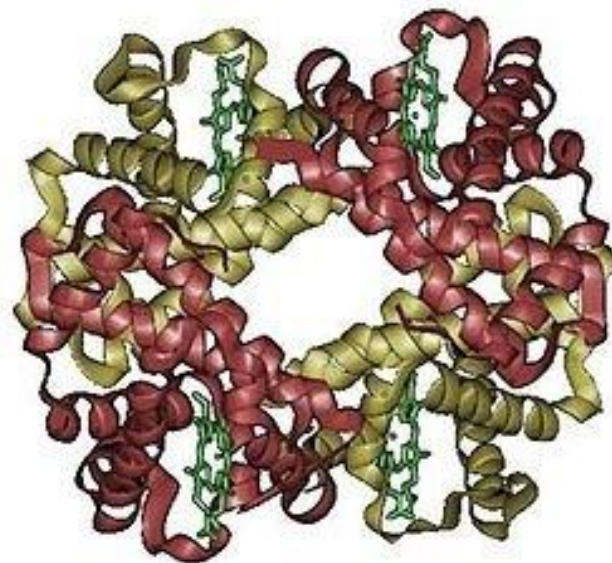
$$P, V, N, T, U, S, F, G \dots$$

Termodynamik

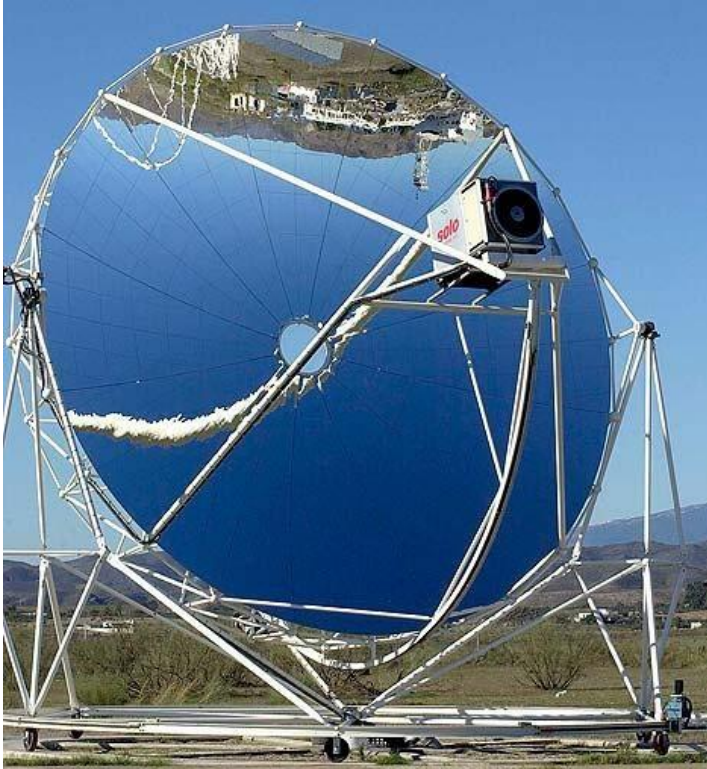
Hur påverkas diamants stabilitet
av tryckförändringar ?



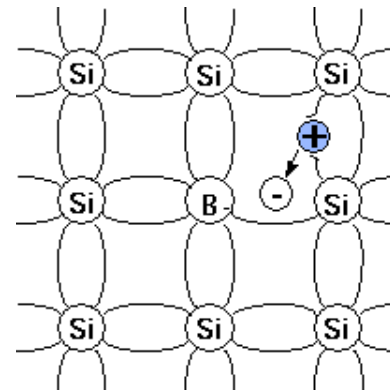
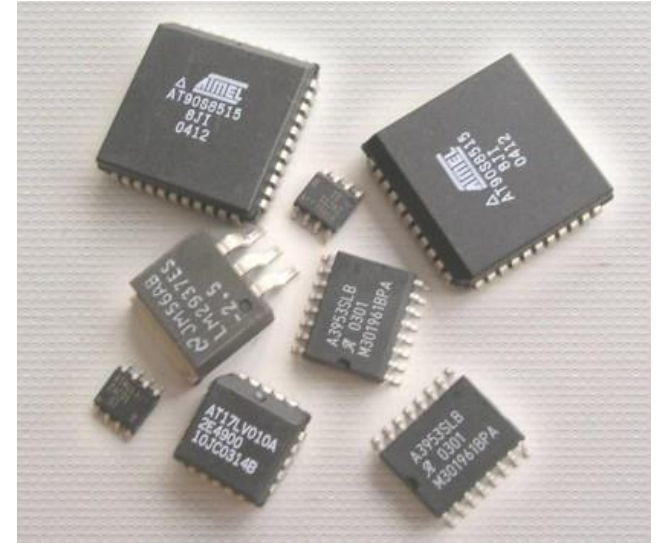
Hur blir man koloxidförgiftad ?



Hur omvandlas värme till elenergi i en Stirlingmotor ?



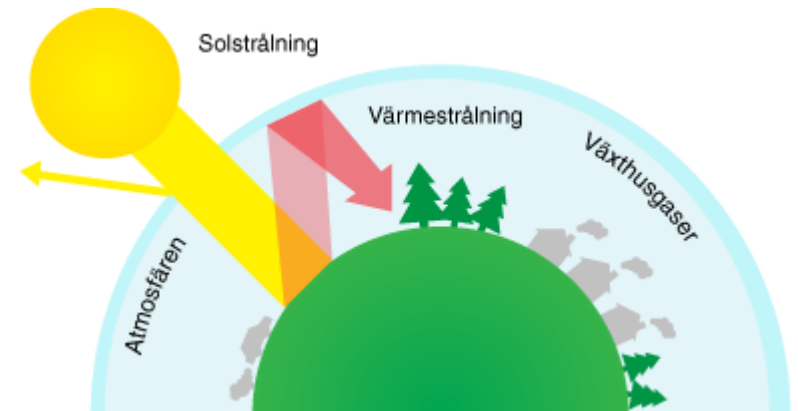
Vad händer när man dopar halvledare ?



Hur fungerar
kompressorkylskåpet ?



Vad är principen bakom
växthuseffekten ?



Smälter isen under skridskon ?



Kan vi förstå stabiliteten av
stjärnor ?



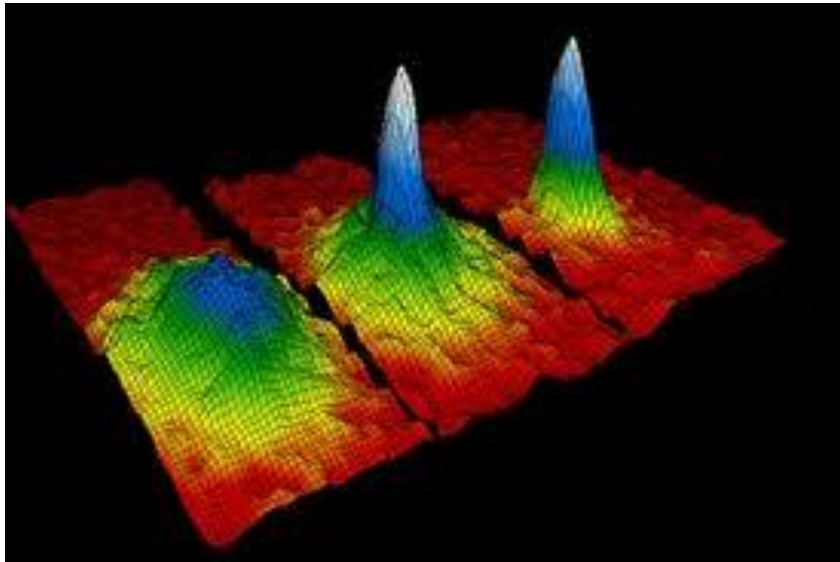
När fryser kylarvätskan ?



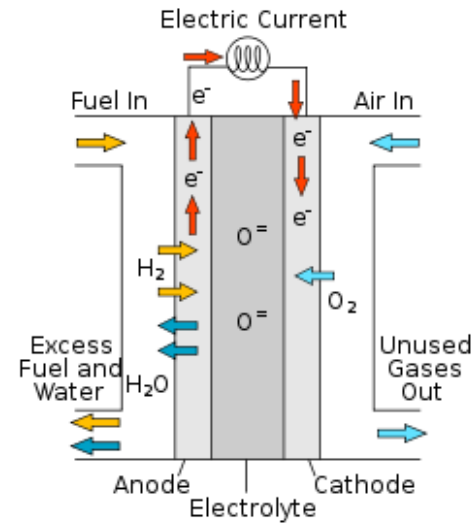
Kan vi förstå egenskaperna för elektroner i en metall ?



Hur bildas ett koherent kvantkondensat av atomer ?



Hur fungerar en bränslecell ?



Kurskoder

Chalmers-kurs:

FTF140 Termodynamik och statistisk mekanik

GU-kurs:

FYP300 Statistisk fysik

Kursbok

Daniel V. Schroeder

An Introduction to Thermal Physics

Tre delar

1. **Grundläggande termodynamik och statistisk mekanik**
Kap 1-3 i Schroeder
2. **Termodynamik med tillämpningar**
Kap 4-5 i Schroeder
3. **Statistisk mekanik med tillämpningar**
Kap 6-7 i Schroeder

16 föreläsningar och övningar

1. **Grundläggande termodynamik och statistisk mekanik**
F/Ö 1-4
2. **Termodynamik med tillämpningar**
F/Ö 5-9
3. **Statistisk mekanik med tillämpningar**
F/Ö 10-16

Hjälp

Arbetsplan 1-16

Sammanfattning

Examination

1. **Skriftlig tentamen**
2. **Två duggor**
3. **En experimentell laboration**

Kurshemsida

Canvas

Termodynamik och statistisk mekanik

FTF140/FYP300

lp1HT19

Fri partikel i en låda

Klassisk beskrivning

$$E_{cl} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) = \frac{p^2}{2m}$$

$$\overline{E_{cl}} = 3 \frac{kT}{2}$$

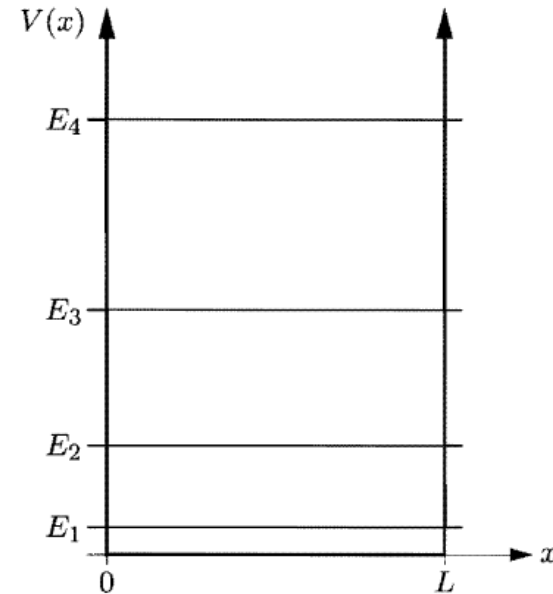
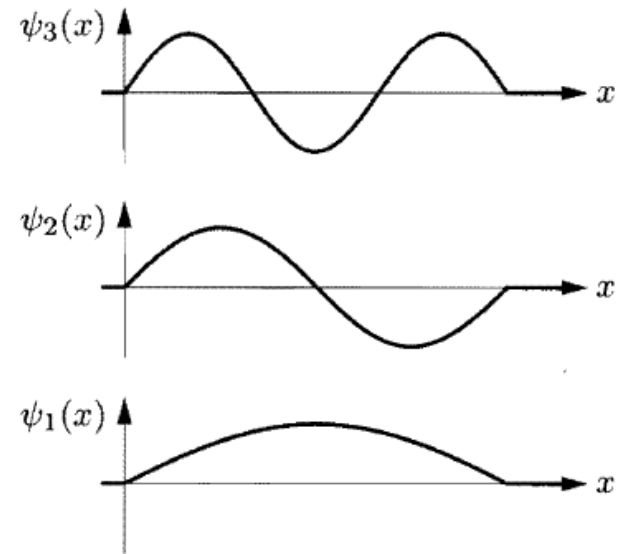
Kvantmekanisk beskrivning

$$E_{n_x n_y n_z} = \frac{1}{2m} \left(\frac{h}{2L} \right)^2 (n_x^2 + n_y^2 + n_z^2)$$

$$n_x, n_y, n_z \in \{1, 2, 3, \dots\}$$

Typisk energiuppsplittring

$$k\theta_{trans} \equiv \frac{1}{2m} \left(\frac{h}{2L} \right)^2$$



Vibrerande molekyl

Klassisk beskrivning

$$E_{cl} = \frac{p^2}{2\mu} + \frac{k_s}{2}q^2 ; \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$\overline{E_{cl}} = 2 \frac{kT}{2}$$

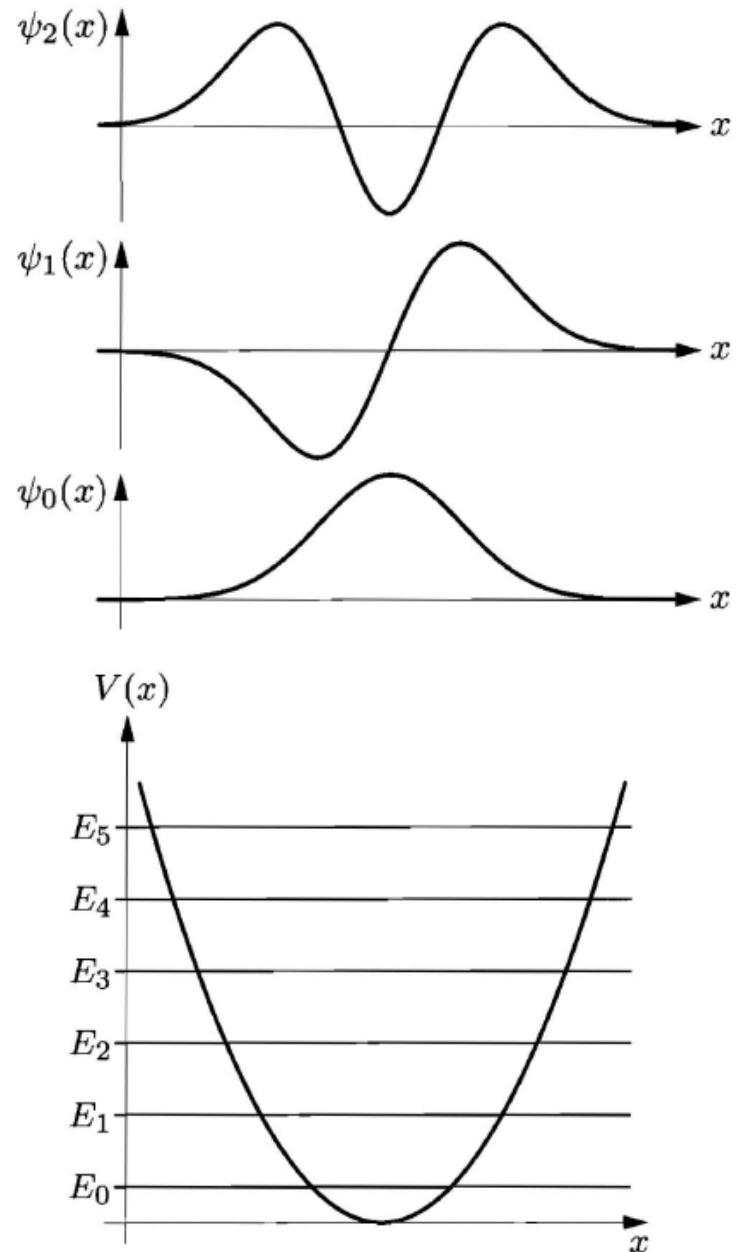
Kvantmekanisk beskrivning

$$E_n = \left(n + \frac{1}{2}\right)hf ; \quad f = \frac{1}{2\pi} \sqrt{\frac{k_s}{\mu}}$$

$$n = 0, 1, 2, \dots$$

Typisk energiuppsplittring

$$k\theta_{vib} \equiv hf$$

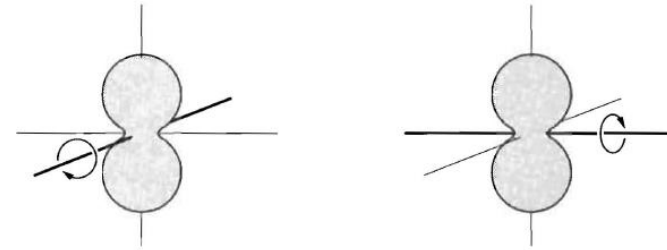


Roterande molekyl

Klassisk beskrivning

$$E_{cl} = \frac{1}{2I}(J_x^2 + J_y^2) ; \quad I = \mu R_0^2$$

$$\overline{E_{cl}} = 2 \frac{kT}{2}$$



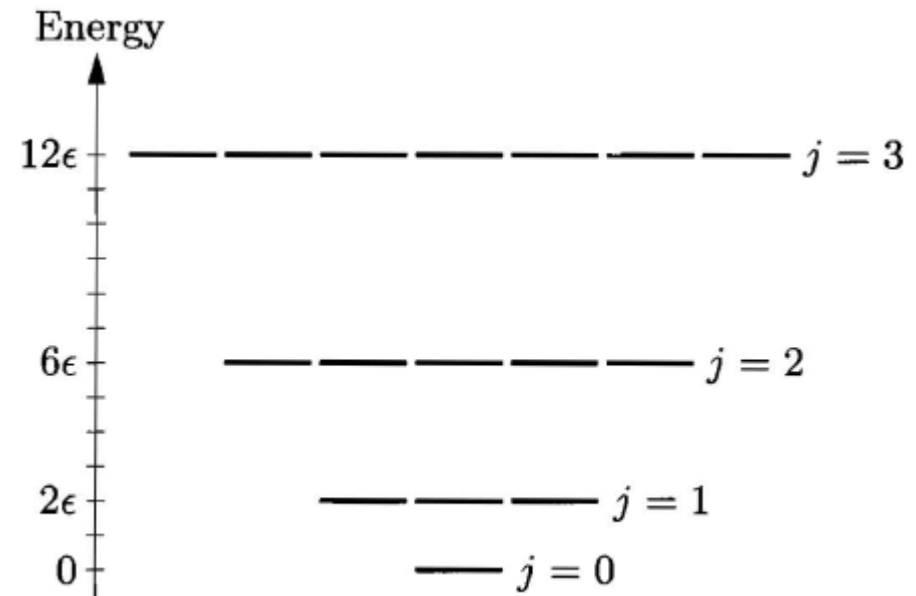
Kvantmekanisk beskrivning

$$E_j = \frac{\hbar^2}{2I}j(j+1) , \quad g_j = 2j+1$$

$$j = 0, 1, 2, \dots$$

Typisk energiuppsplittring

$$k\theta_{rot} \equiv \frac{\hbar^2}{2I}$$



Typisk energiuppsplittring

	θ_{trans} (K)	θ_{vib} (K)	θ_{rot} (K)
H ₂	$12 \cdot 10^{-19}$	$6.3 \cdot 10^3$	85
O ₂	$0.75 \cdot 10^{-19}$	$2.3 \cdot 10^3$	2.1
N ₂	$0.85 \cdot 10^{-19}$	$3.4 \cdot 10^3$	2.9
CO	$0.85 \cdot 10^{-19}$	$3.1 \cdot 10^3$	2.8
NO	$0.80 \cdot 10^{-19}$	$2.7 \cdot 10^3$	2.4

med $L=1\text{m}$

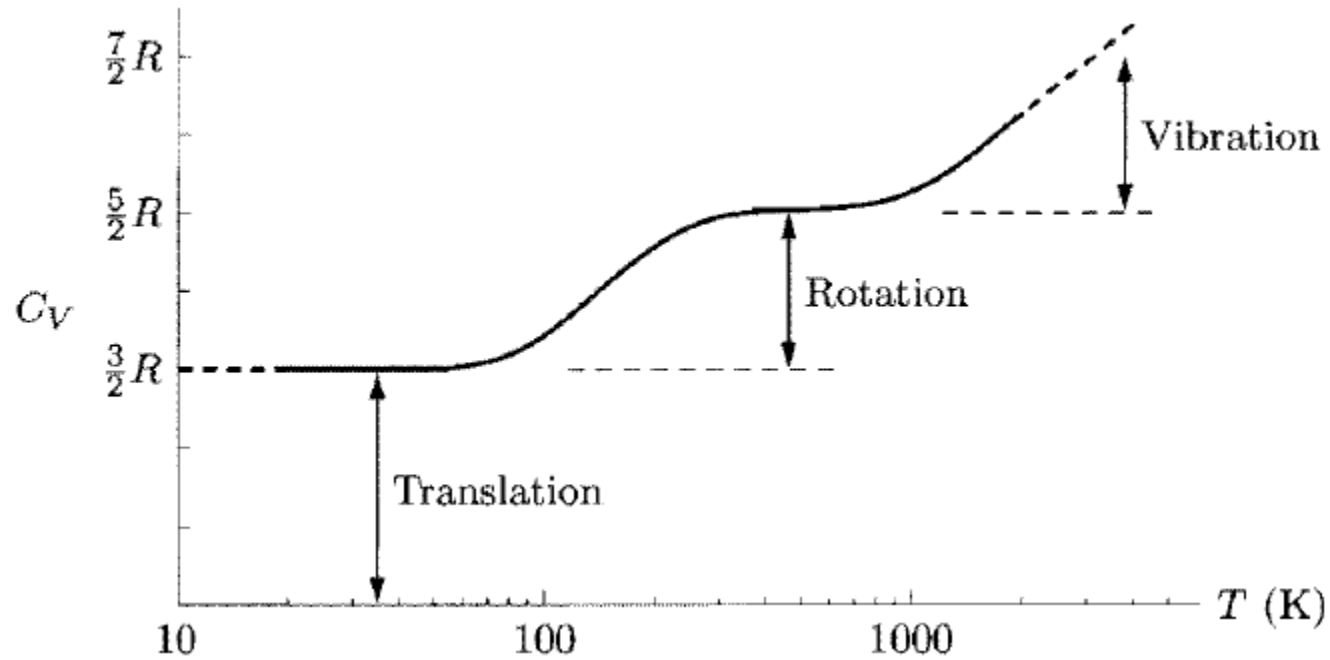
Vid rumstemperatur:

Translationsrörelsen: **alltid** klassisk

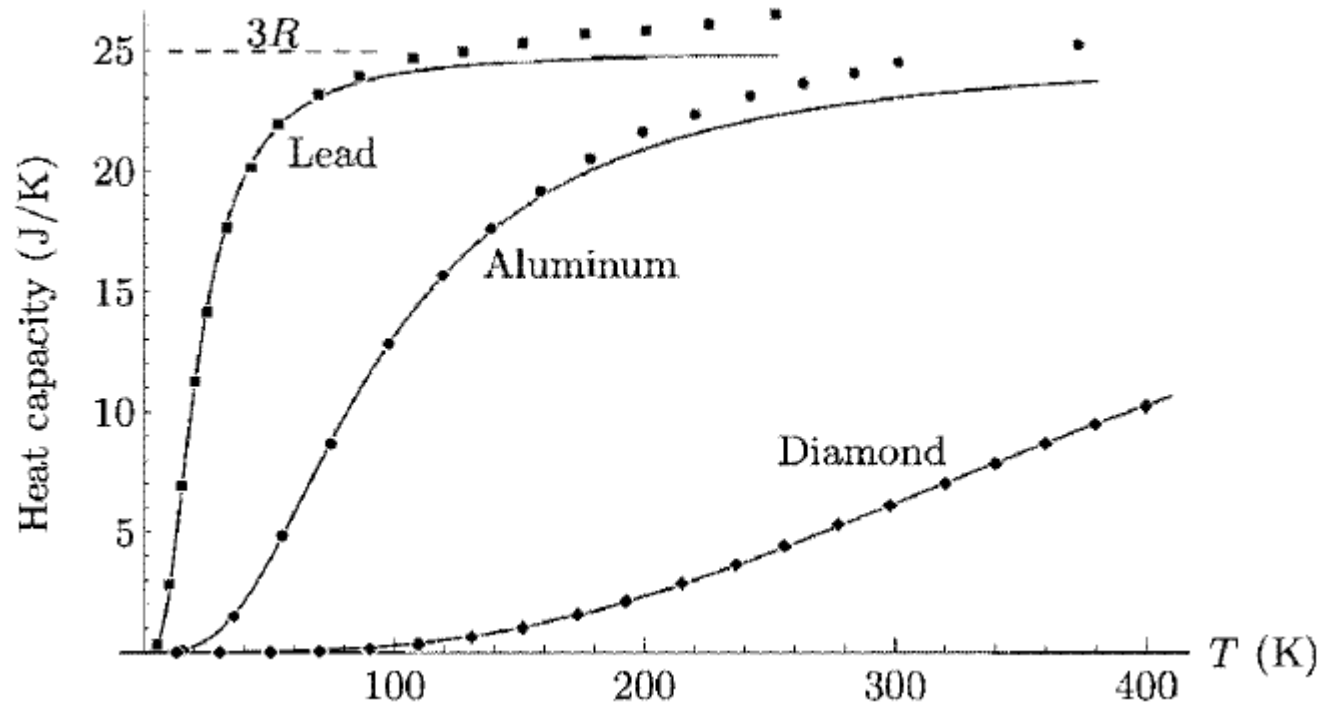
Vibrationsrörelsen: kvantmekanisk

Rotationsrörelsen: klassisk

Experimentell värmekapacitivitet för H₂

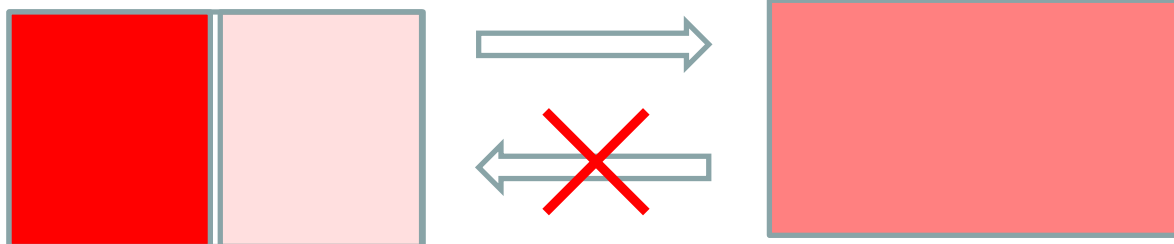


Experimentell värmekapacitivitet för fasta ämnen

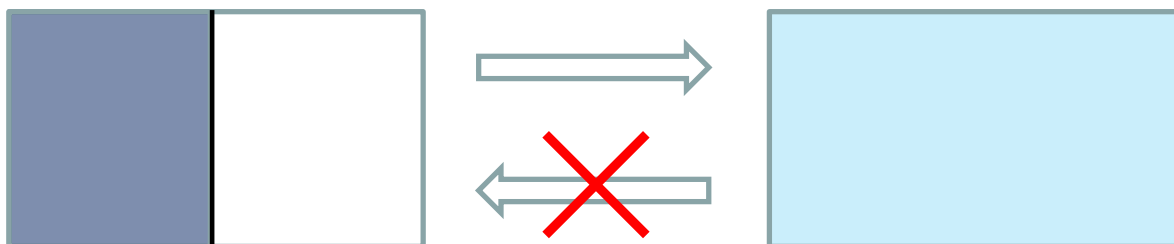


Irreversibla processer

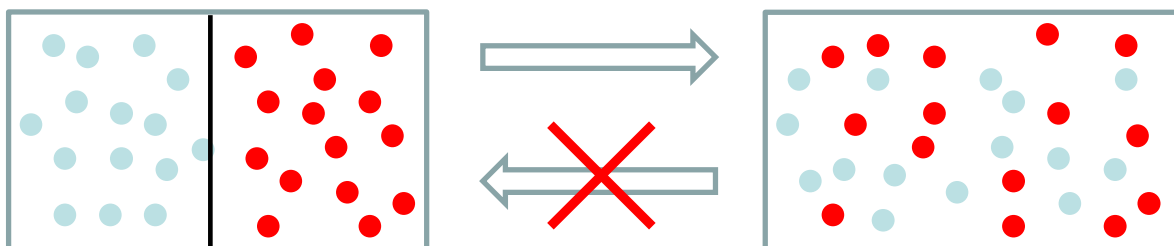
Temperaturutjämnning



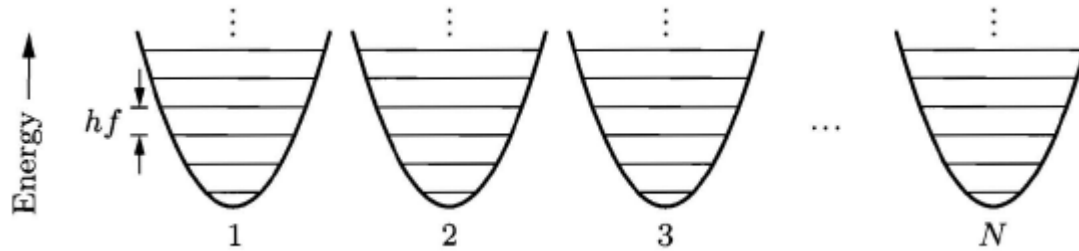
Fri expansion



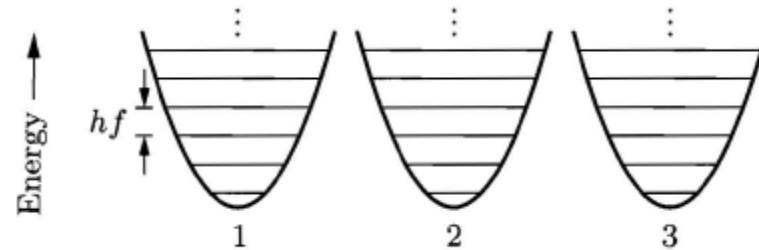
Blandning



N st harmoniska oscillatorer



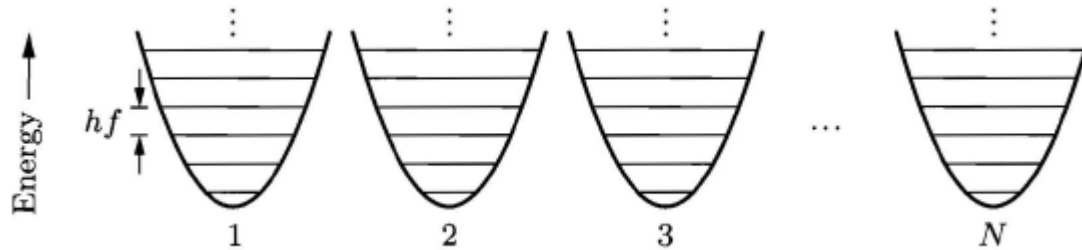
3 st harmoniska oscillatorer



Oscillator:	#1	#2	#3
Energy:	0	0	0
	1	0	0
	0	1	0
	0	0	1
	2	0	0
	0	2	0
	0	0	2
	1	1	0
	1	0	1
	0	1	1

Oscillator:	#1	#2	#3
Energy:	3	0	0
	0	3	0
	0	0	3
	2	1	0
	2	0	1
	1	2	0
	0	2	1
	1	0	2
	0	1	2
	1	1	1

Harmoniska oscillatorer



Multipliciteten för en uppsättning av N identiska harmoniska oscillatorer ges av uttrycket

$$\Omega(N, q) = \frac{(q + N - 1)!}{q!(N - 1)!}$$

där q är totala antalet energikvanta för systemet,

$$E = qhf + E_0 ; \quad E_0 = (N/2)hf$$

Uttryck för stora system:

$$\Omega(N, q) \rightarrow \left(\frac{q+N}{q}\right)^q \left(\frac{q+N}{N}\right)^N \quad \text{om } q, N \gg 1$$

$$\Omega(N, q) \rightarrow \left(\frac{eq}{N}\right)^N \quad \text{om } q \gg N \gg 1$$

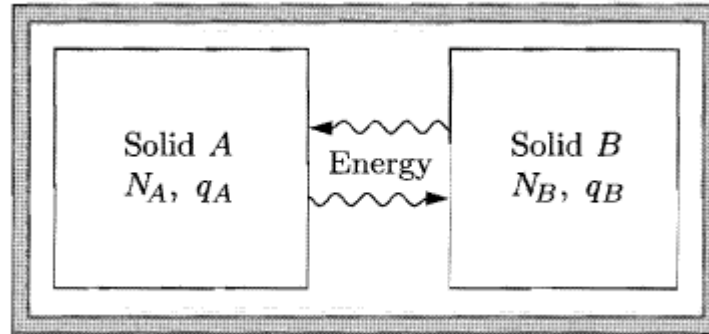
$$\Omega(N, q) \rightarrow \left(\frac{eN}{q}\right)^q \quad \text{om } N \gg q \gg 1$$

System i termisk kontakt

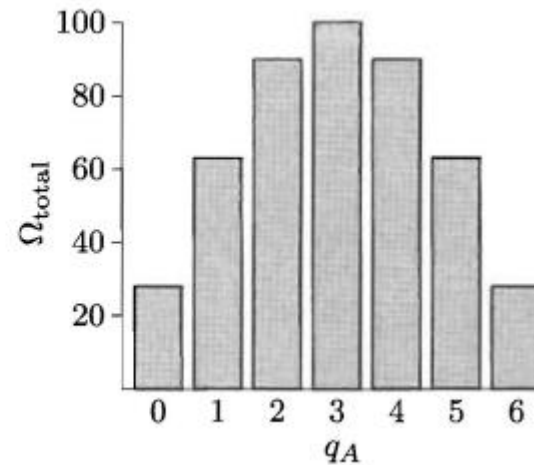
$$N_A = 3$$

$$N_B = 3$$

$$q_A + q_B = q_{total} = 6$$



q_A	Ω_A	q_B	Ω_B	$\Omega_{total} = \Omega_A \Omega_B$
0	1	6	28	28
1	3	5	21	63
2	6	4	15	90
3	10	3	10	100
4	15	2	6	90
5	21	1	3	63
6	28	0	1	28
				462 = $\binom{6+6-1}{6}$

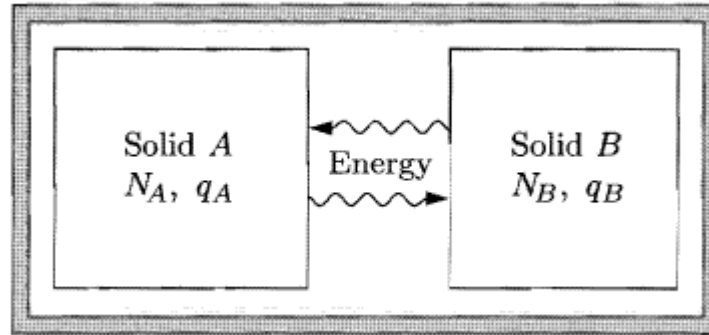


System i termisk kontakt

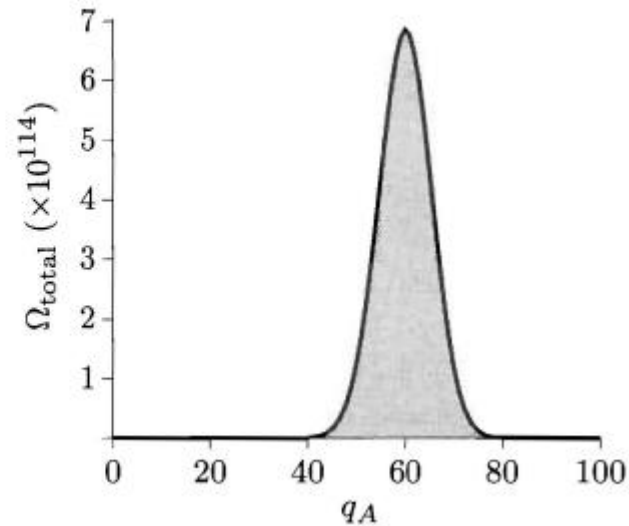
$$N_A = 300$$

$$N_B = 200$$

$$q_A + q_B = q_{total} = 100$$



q_A	Ω_A	q_B	Ω_B	Ω_{total}
0	1	100	2.8×10^{81}	2.8×10^{81}
1	300	99	9.3×10^{80}	2.8×10^{83}
2	45150	98	3.1×10^{80}	1.4×10^{85}
3	4545100	97	1.0×10^{80}	4.6×10^{86}
4	3.4×10^8	96	3.3×10^{79}	1.1×10^{88}
⋮	⋮	⋮	⋮	⋮
59	2.2×10^{68}	41	3.1×10^{46}	6.8×10^{114}
60	1.3×10^{69}	40	5.3×10^{45}	6.9×10^{114}
61	7.7×10^{69}	39	8.8×10^{44}	6.8×10^{114}
⋮	⋮	⋮	⋮	⋮
100	1.7×10^{96}	0	1	1.7×10^{96}
				9.3×10^{115}

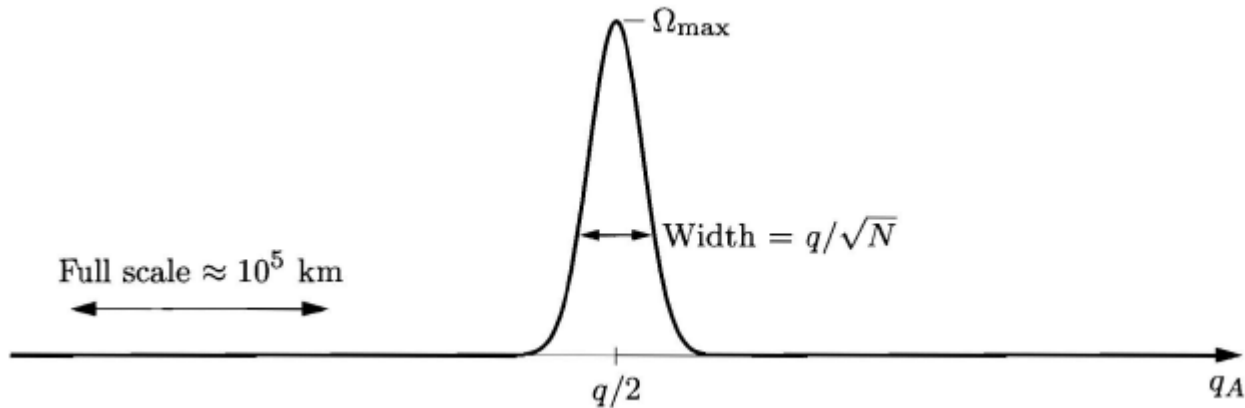
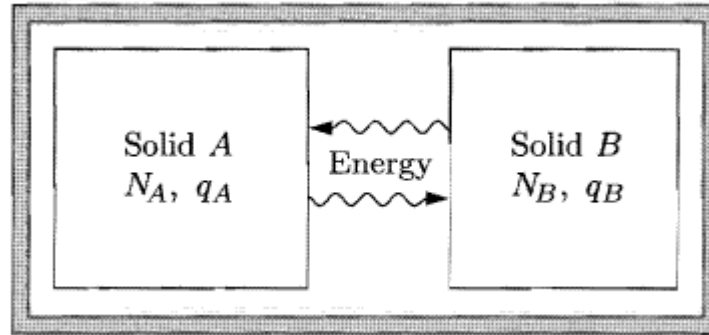


System i termisk kontakt

$$N_A = \text{large}$$

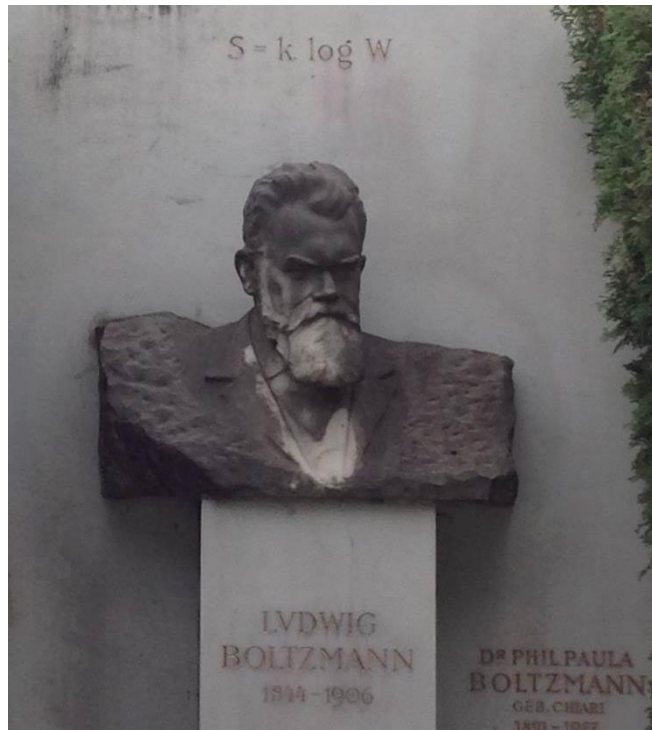
$$N_B = \text{large}$$

$$q_A + q_B = q_{\text{total}} = \text{large}$$



Konsekvens av det grundläggande antagandet (Termodynamikens andra huvudsats)

För ett stort system i jämvikt gäller att det kommer att befinna sig i det mest sannolika makrotillståndet (med försumbara fluktuationer från detta tillstånd).



Boltzmann's definition av entropin

$$S \equiv k \ln \Omega$$

Zentralfriedhof (Central Cemetery) in Vienna, Austria





Boltzmann's definition av entropin

$$S \equiv k \ln \Omega$$

För ett isolerat system gäller att entropin har en tendens att öka

$$\Delta S \geq 0$$

Vid jämvikt kommer systemet befinna sig i det makrotillstånd med maximal entropi (med, för stora system, försumbara fluktuationer).

Termodynamikens huvudsatser

Första huvudsatsen

$$\Delta U = Q + W$$

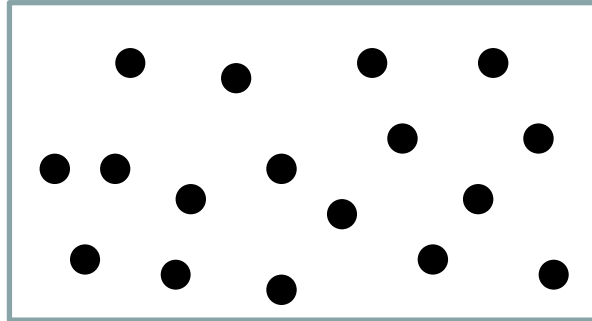
Isolerat system: $\Delta U = 0$

Andra huvudsatsen

$$\Delta S \geq \frac{Q}{T}$$

Isolerat system: $\Delta S \geq 0$

Klassisk idealgas



Multipliciteten för en gas av N icke-växelverkande identiska atomer med massan m i den klassiska gränsen ges av uttrycket

$$\Omega(N, V, U) = \frac{1}{N!} \frac{\pi^{3N/2}}{(3N/2)!} \frac{V^N}{h^{3N}} (2mU)^{3N/2} \equiv f(N) V^N U^{3N/2}$$

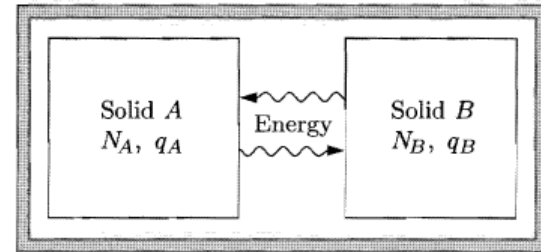
där V och U är systemets volym respektive energi.

Entropi

$$S(U, V, N) \equiv k \ln \Omega(U, V, N)$$

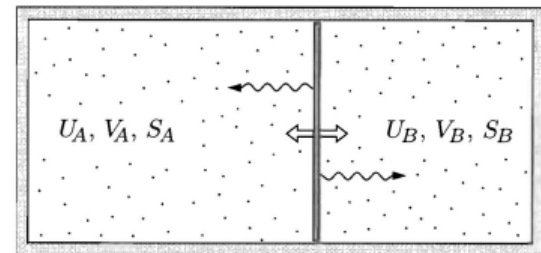
Temperatur

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



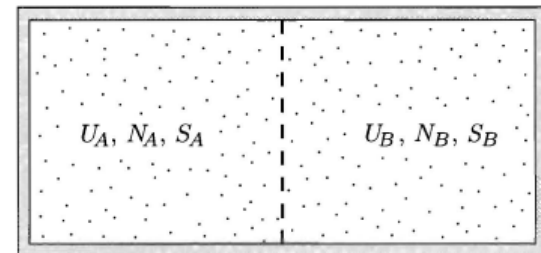
Tryck

$$\frac{P}{T} \equiv \left(\frac{\partial S}{\partial V} \right)_{U, N}$$



Kemisk potential

$$\frac{\mu}{T} \equiv - \left(\frac{\partial S}{\partial N} \right)_{U, V}$$



Termodynamiska identiteten

$$dS = \frac{1}{T}dU + \frac{P}{T}dV - \frac{\mu}{T}dN$$

Sammanfattning

typ av växelverkan	överförd storhet	drivande "kraft"	matematisk definition
termisk	energi	temperatur	$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_{V,N}$
mekanisk	volym	tryck	$\frac{P}{T} = \left(\frac{\partial S}{\partial V}\right)_{U,N}$
diffusiv	partiklar	kemisk potential	$\frac{\mu}{T} = -\left(\frac{\partial S}{\partial N}\right)_{U,V}$