

English Summary:

4.4 Equilibrium Statistics: ideal Fermi gas

thermodyn. equil.: minimum Shannon info. $I(\hat{\rho}) = -\text{tr}(\hat{\rho} \ln \hat{\rho})$

under constraints $\text{tr} \hat{\rho} = 1, \text{tr}(\hat{\rho} \hat{M}^v) = \langle M^v \rangle$

canonical statistical op. $\hat{\rho} = Z^{-1} e^{-\beta \hat{H}}$, partition fct. $Z = \text{tr} e^{-\beta \hat{H}}, \beta = \frac{1}{kT}$

grandcanonical statist. op. $\hat{\rho} = \Xi^{-1} e^{-\beta(\hat{H} - \mu \hat{N})}$

Fermi distribution

$$\langle N_j \rangle = \frac{1}{\exp\left[\frac{E_j - \mu}{kT}\right] + 1}$$

grandcanonical Zustandssumme:

$$\ln \Xi = \sum_j \ln [1 + \zeta e^{-\beta E_j}] \quad (\zeta = e^{\beta \mu} \text{ Fugazität})$$

$$\approx (2S+1) \frac{4\pi V}{h^3} \int_0^\infty dp p^2 \ln [1 + \zeta e^{-\beta \frac{p^2}{2m}}]$$

$$\text{part. Int.} = (2S+1) \frac{4\pi V}{h^3} \left\{ \frac{p^3}{3} \ln [1 + \zeta e^{-\beta \frac{p^2}{2m}}] \Big|_0^\infty - \int_0^\infty dp \frac{p^3}{3} \frac{(-\frac{\beta p}{m}) \zeta e^{-\beta \frac{p^2}{2m}}}{1 + \zeta e^{-\beta \frac{p^2}{2m}}} \right\}$$

$$= \frac{2}{3} (2S+1) \frac{4\pi V}{h^3} \int_0^\infty dp p^2 \frac{\frac{\beta p^2}{2m}}{\frac{1}{\zeta} \exp\left\{\frac{\beta p^2}{2m}\right\} + 1}$$

$$= \frac{2}{3} \beta (2S+1) \frac{4\pi V}{h^3} \int_0^\infty dp p^2 \langle N(p) \rangle E(p)$$

$$\text{diskret} = \frac{2}{3} \beta \sum_j \langle N_j \rangle E_j$$

$$= \frac{2}{3} \beta U \quad \text{innere Energie } U$$

$$\Rightarrow pV = kT \ln \Xi = \frac{2}{3} U$$

(i) gilt auch für klass. ideales Gas!

$$\left. \begin{aligned} pV &= \bar{N} kT \\ U &= \frac{3}{2} \bar{N} kT \end{aligned} \right\} pV = \frac{2}{3} U$$

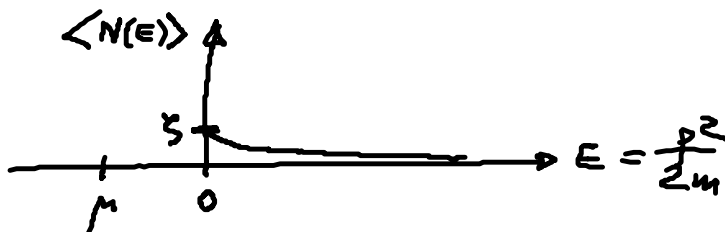
(ii) gilt auch für Bose-Gas (s. später)

also unabh. von der speziellen Statistik!

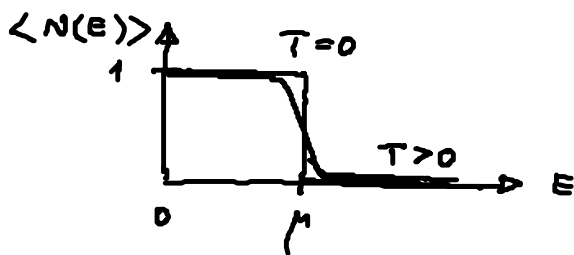
a) Klass. Grenzfall der Fermi-Verteilung: Nichtentartung

$$\langle N(p) \rangle = \frac{1}{\frac{1}{\zeta} \exp\left(\frac{p^2}{2mkT}\right) + 1} \approx \zeta \exp\left(-\frac{p^2}{2mkT}\right) \quad \text{Maxwell-Boltzmann}$$

für $\zeta = e^{\frac{\mu}{kT}} \ll 1$, d.h. $\mu < 0$ (stark verdünnt)



b) Nichtklass. Grenzfall („Fermi-Entartung“)



$\zeta \gg 1$ (hohe Dichte)

Gesamte Teilchenzahl:

$$\bar{N} = \frac{4\pi V}{h^3} (2s+1) \int_0^{\infty} dp p^2 \frac{1}{\exp\left\{\frac{\left(\frac{p^2}{2m} - \mu\right)}{kT}\right\} + 1}$$

Innere Energie:

$$U = \frac{4\pi V}{h^3} (2s+1) \int_0^{\infty} dp p^2 \frac{\frac{p^2}{2m}}{\exp\left\{\frac{\left(\frac{p^2}{2m} - \mu\right)}{kT}\right\} + 1}$$

Substitution:

$$\frac{p^2}{2mkT} = \eta, \quad p dp = mkT d\eta, \quad \frac{\mu}{kT} = \eta (= -\alpha)$$

(reduzierte Fermi-Niveaus)

$$\bar{N} = \frac{4\pi V}{h^3} \frac{2s+1}{2} (2mkT)^{3/2} \int_0^\infty d\eta \frac{\eta^{1/2}}{e^{\eta-\eta} + 1}$$

$$\mu = \frac{4\pi V}{h^3} \frac{2s+1}{2} (2mkT)^{3/2} kT \int_0^\infty d\eta \frac{\eta^{3/2}}{e^{\eta-\eta} + 1}$$

Def. Fermi-Dirac-Integral der Ordnung s

$$F_s(\eta) := \frac{1}{\Gamma(s+1)} \int_0^\infty d\eta \frac{\eta^s}{e^{\eta-\eta} + 1} \quad (s > 0)$$

Entwicklung für $\eta \gg 1$ ($\triangleq s \gg 1$, d.h. Entartung)

$$\begin{aligned} \Gamma(s+1) F_s(\eta) &\stackrel{\text{part. Int.}}{=} \frac{1}{s+1} \int_0^\infty d\eta \underbrace{\frac{d}{d\eta} (\eta^{s+1})}_{u'} \underbrace{\frac{1}{e^{\eta-\eta} + 1}}_v \\ &= \frac{1}{s+1} \left[\frac{\eta^{s+1}}{e^{\eta-\eta} + 1} \right]_0^\infty + \frac{1}{s+1} \int_0^\infty d\eta \eta^{s+1} \frac{e^{-\eta}}{(e^{\eta-\eta} + 1)^2} \end{aligned}$$

$$\begin{aligned} &\stackrel{x = \eta - \eta}{=} \frac{1}{s+1} \int_{-\infty}^\infty dx (x+\eta)^{s+1} \frac{e^x}{(e^x + 1)^2} \\ &\quad \eta \gg 1 \end{aligned}$$

Entwicklung $(x+\eta)^{s+1} \approx \eta^{s+1} + (s+1)\eta^s x + \frac{s(s+1)}{2}\eta^{s-1} x^2 + \dots$

$$\begin{aligned} \Gamma(s+1) F_s(\eta) &\approx \underbrace{\frac{\eta^{s+1}}{s+1} \int_{-\infty}^\infty dx \frac{e^x}{(e^x + 1)^2}}_{\left[-\frac{1}{e^x + 1} \right]_{-\infty}^\infty = 1} + \underbrace{\eta^s \int_{-\infty}^\infty dx \frac{x e^x}{(e^x + 1)^2}}_{= 0, \text{ da Integrand ungerade}} + \underbrace{\frac{s}{2} \eta^{s-1} \int_{-\infty}^\infty dx \frac{x^2 e^x}{(e^x + 1)^2}}_{= \frac{\pi^2}{3}} \end{aligned}$$

$$\Rightarrow F_s(\eta) = \frac{1}{\Gamma(s+1)} \left[\frac{\eta^{s+1}}{s+1} + s \frac{\pi^2}{6} \eta^{s-1} + O(\eta^{s-3}) \right]$$

speziell:

$$F_{1/2}(\eta) \approx \frac{2}{\sqrt{\pi}} \left[\frac{\eta^{3/2}}{3/2} + \frac{\pi^2}{12} \eta^{-1/2} \right]$$

$$F_{3/2}(\eta) \approx \frac{4}{3\sqrt{\pi}} \left[\frac{\eta^{5/2}}{5/2} + \frac{\pi^2}{4} \eta^{1/2} \right]$$

$$\begin{aligned} \bar{N} &= \frac{4\pi V}{h^3} \frac{2S+1}{2} (2m kT)^{3/2} \left[\frac{2}{3} \left(\frac{m}{kT} \right)^{3/2} + \frac{\pi^2}{12} \left(\frac{m}{kT} \right)^{-1/2} \right] \\ &= \frac{2}{3} \frac{4\pi V}{h^3} \frac{2S+1}{2} (2m \mu)^{3/2} \left[1 + \frac{\pi^2}{8} \left(\frac{kT}{\mu} \right)^2 \right] \quad (1) \end{aligned}$$

Halbleiter: $\mu = E_F \Rightarrow n \sim E_F^{3/2}$ Fermi-Niveau

$$\begin{aligned} U &= \frac{4\pi V}{h^3} \frac{2S+1}{2} (2m)^{3/2} (kT)^{5/2} \left[\frac{2}{5} \left(\frac{m}{kT} \right)^{5/2} + \frac{\pi^2}{4} \left(\frac{m}{kT} \right)^{1/2} \right] \\ &= \frac{2}{5} \frac{4\pi V}{h^3} \frac{2S+1}{2} (2m)^{3/2} \mu^{5/2} \left[1 + \frac{5\pi^2}{8} \left(\frac{kT}{\mu} \right)^2 \right] \end{aligned}$$

$$\Rightarrow \boxed{ \begin{aligned} U &= \frac{3}{5} \bar{N} E_F \left[1 + \frac{5\pi^2}{12} \left(\frac{kT}{E_F} \right)^2 \right] && \text{kalor. Zustandsgl.} \\ pV &= \frac{2}{3} U = \frac{2}{5} \bar{N} E_F \left[1 + \frac{5\pi^2}{12} \left(\frac{kT}{E_F} \right)^2 \right] && \text{therm. Zustandsgl.} \end{aligned} }$$

NB: Metalle: $E_F = \mu(T=0, \bar{N}, V)$, Halbleiter $E_F = \mu(T, \bar{N}, V)$

Druck des Fermigas ist um einen Faktor $\sim \frac{E_F}{kT}$ größer als in klass. idealen Gasen ($pV = \bar{N}kT$),
(z.B.: $E_F \approx 1\text{eV} \hat{=} T \sim 10^4\text{K}$!)

Grund: Pauli-Prinzip (eff. Abstoßung der Teilchen)

spezif. Wärme

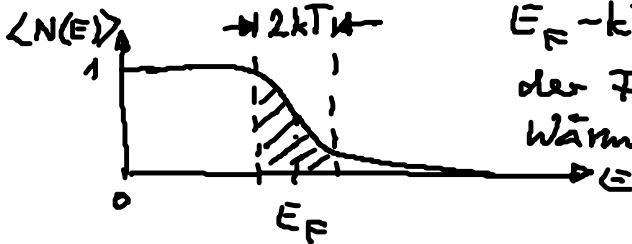
$$C_V = \left(\frac{\partial U}{\partial T} \right)_V = \frac{\pi^2}{2} \bar{N} k \frac{kT}{E_F} \quad \text{Wärme Kapazität}$$

$$C_V = \frac{\pi^2}{2} R \frac{kT}{E_F} \sim T$$

um Faktor $\frac{kT}{E_F}$ kleiner als in klass. idealen Gasen ($C_V = \frac{3}{2} R$),
 bei $T \approx 300 \text{ K}$: $\frac{1}{40}$ kleiner

($R = N_A k$ allg. Gaskonst.)

Grund: Nur Teilchen in der „Aufweichungszone“



$$E_F - kT < E < E_F + kT$$

der Fermi-Verteilung tragen zur spezif. Wärme bei, da nur sie in freie Zustände thermisch angeregt werden können.

Zahl $\Delta N \sim \bar{N} \frac{kT}{E_F}$, jedes hat Energie $\sim kT$

$$\Rightarrow \Delta U \sim \bar{N} \frac{(kT)^2}{E_F} \Rightarrow C_V \sim \bar{N} k \frac{kT}{E_F}$$

Beispiele für entartetes Fermigas:

- Elektronen in Metallen (hohe Dichte!)
- Elektronen in Halbleitern bei hoher Dotierung oder tiefen Temp.

Nichtentartetes Fermigas

(verdünntes, nichtrelativist. Quantengas, z.B. Elektronen in Halbleitern im Normalbereich)

Vor $\zeta = e^{\frac{\mu}{kT}} \ll 1$ d.h. $\mu < 0$, $z = \frac{\mu}{kT} < 0$

Entw. des Fermi-Dirac-Integral nach Potenzen von ζ :

$$F_s(\eta) = \frac{1}{\Gamma(s+1)} \int_0^\infty dy \frac{y^s}{e^{y-\eta} + 1}$$

$$= \frac{1}{\Gamma(s+1)} \int_0^\infty dy y^s \frac{\zeta e^{-y}}{1 + \zeta e^{-y}}$$

$$\approx \frac{1}{\Gamma(s+1)} \left[\underbrace{\int_0^\infty dy y^s e^{-y}}_{\Gamma(s+1)} - \zeta^2 \underbrace{\int_0^\infty dy y^s e^{-2y}}_{\frac{1}{2^{s+1}} \int_0^\infty dz z^s e^{-z}} + \dots \right]$$

$$= e^{\frac{\mu}{kT}} \left[1 - \frac{1}{2^{s+1}} e^{\frac{\mu}{kT}} \right]$$

↑
Boltzmann-Limit

↑
Quantenkorrektur

$$\bar{N} = V N_c F_{1/2} \left(\frac{\mu}{kT} \right) \quad \text{mit Entartungskonz. } N_c := (2s+1) \left(\frac{2\pi m kT}{h^2} \right)^{3/2}$$

$$n = \frac{\bar{N}}{V} \approx N_c e^{\frac{\mu}{kT}} \left[1 - \frac{1}{2^{3/2}} e^{\frac{\mu}{kT}} \right]$$

Vollständige Nichtentartung
(klass. Maxwell-Boltzmann)

$$\mu \approx N_c e^{\frac{\mu}{kT}} \quad (\ll N_c)$$

$$U = V N_c \frac{3}{2} kT F_{3/2} \left(\frac{\mu}{kT} \right) \approx \frac{3}{2} kT V N_c e^{\frac{\mu}{kT}} \left[1 - \frac{1}{2^{5/2}} e^{\frac{\mu}{kT}} \right]$$

Elim. von μ durch \bar{N} (selbstkonsistent):

$$U \approx \frac{3}{2} kT \bar{N} \left[1 + \frac{1}{2^{5/2}} \frac{\bar{N}}{V N_c(T)} \right]$$

kalor. Zustandsgl.

$$pV = \frac{2}{3} U = kT \bar{N} \left[1 + \frac{1}{2^{5/2}} \frac{\bar{N}}{V N_c(T)} \right]$$

therm. Zustandsgl.

$$p v = RT \left(1 + \frac{1}{2^{5/2}} \frac{N_A}{v N_c(T)} \right)$$

v Molvol.

N_A Avogadro-Konst.

klass. ideales Gas

↑
Fermi-Abstoßung
(erhöhter Druck)