English Summary:

4.4 Equilibrium Statistics: ideal Fermi gas

thermodyn. equil.: minimum Shannon info. $I(\hat{\varrho}) = \mathrm{tr}(\hat{\varrho} \ln \hat{\varrho})$

under constraints $\mathrm{tr}\,\hat{\varrho} = 1$, $\mathrm{tr}(\hat{\varrho}\hat{M}^\nu) = \langle M^\nu \rangle$

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

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

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

großkanon. Zustandssumme:

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

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

$$\overset{\text{part. Int.}}{=} (2S+1) \frac{4\pi V}{h^3} \left\{ \underbrace{\frac{p^3}{3} \ln\left[1 + \zeta e^{-\beta\frac{p^2}{2m}}\right]_0^\infty}_{0} - \int_0^\infty dp \frac{p^3}{3} \frac{\left(-\frac{\beta p}{m}\right)\zeta e^{-\beta\frac{p^2}{2m}}}{1 + \zeta e^{-\beta\frac{p^2}{2m}}} \right\}$$

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

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

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

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

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

(i) gilt auch für <u>klass.</u> ideales Gas!

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

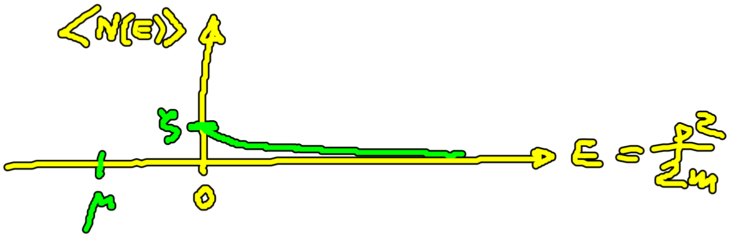
(ii) gilt auch für Bose-Gas (s. später)

also unabh. von der speziellen Statistik!

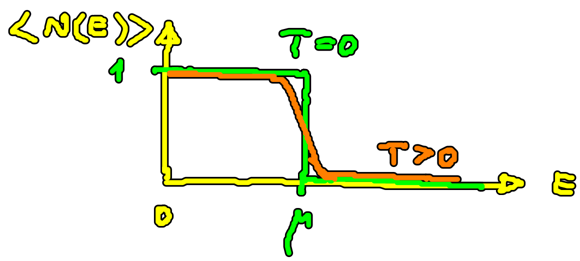
a) Klass. Grenzfall der Fermi-Verteilung: Nichtentartung

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

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



b) Nichtklass. Grenzfall („<u>Fermi-Entartung</u>")



$\boxed{z \gg 1}$ (hohe Dichte)

Gesamte Teilchenzahl:

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

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:

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

(reduzierte Fermi-Niveau)

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

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

Def. <u>Fermi-Dirac-Integral</u> der Ordnung s

$$F_s(\eta) := \frac{1}{\Gamma(s+1)}\int_0^\infty dy\,\frac{y^s}{e^{y-\eta}+1} \qquad (s>0)$$

<u>Entwicklung für $\eta \gg 1$</u> ($\hat{=}\ \xi \gg 1$, d.h. Entartung)

$$\Gamma(s+1)\,F_s(\eta) \overset{\text{part. Int.}}{=} \frac{1}{s+1}\int_0^\infty dy\,\underbrace{\frac{d}{dy}\left(y^{s+1}\right)}_{u'}\,\underbrace{\frac{1}{e^{y-\eta}+1}}_{v}$$

$$= \frac{1}{s+1}\underbrace{\left[\frac{y^{s+1}}{e^{y-\eta}+1}\right]_0^\infty}_{0} + \frac{1}{s+1}\int_0^\infty dy\,y^{s+1}\,\frac{e^{y-\eta}}{(e^{y-\eta}+1)^2}$$

$$\overset{x=y-\eta}{=} \frac{1}{s+1}\int_{\cancel{-\eta}\ (\eta\gg1)\ \to\ -\infty}^{\infty} dx\,(x+\eta)^{s+1}\,\frac{e^x}{(e^x+1)^2}$$

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

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

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

speziell:

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

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

$$\bar{N} = \frac{4\pi V}{h^3}\,\frac{2S+1}{2}(2mkT)^{3/2}\left[\frac{2}{3}\left(\frac{\mu}{kT}\right)^{3/2} + \frac{\pi^2}{12}\left(\frac{\mu}{kT}\right)^{-1/2}\right]$$

$$= \frac{2}{3}\,\frac{4\pi V}{h^3}\,\frac{2S+1}{2}(2m\mu)^{3/2}\left[1 + \frac{\pi^2}{8}\left(\frac{kT}{\mu}\right)^2\right] \qquad (1)$$

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

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

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

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

<u>kalor. Zustandsgl.</u>

<u>therm. Zustandsgl.</u>

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

Druck des Fermigases ist um einen Faktor $\sim \frac{E_F}{kT}$ größer als in <u>klass.</u> idealen Gasen ($pV = \bar{N}kT$)
(z.B.: $E_F \approx 1\,\mathrm{eV} \;\hat{=}\; T \sim 10^4\,\mathrm{K}$!)
Grund: <u>Pauli-Prinzip</u> (eff. Abstoßung der Teilchen)

spezif. Wärme

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

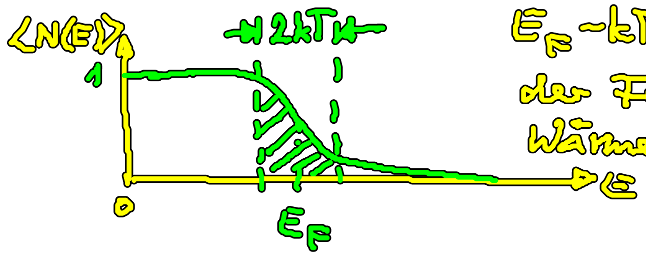
$$\boxed{c_V = \frac{\pi^2}{2} R \frac{kT}{E_F} \sim T}$$

um Faktor $\frac{kT}{E_F}$ kleiner als in klass. idealen Gasen $\left(c_V = \frac{3}{2} R\right)$, bei $T \approx 300\,K$: $\frac{1}{40}$ 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. $\boxed{\zeta = e^{\frac{\mu}{kT}} \ll 1}$ d.h. $\mu < 0$, $\eta = \frac{\mu}{kT} < 0$

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

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

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

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

$$= \underset{\substack{\uparrow\\ \text{Boltzmann-Limit}}}{e^{\frac{\mu}{kT}}}\Big[1 - \underset{\substack{\uparrow\\ \text{Quantenkorrektur}}}{\frac{1}{2^{s+1}}} e^{\frac{\mu}{kT}}\Big]$$

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

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

Vollständige Nichtentartung (klass. Maxwell-Boltzmann) $\boxed{n \approx N_c \underbrace{e^{\frac{E_F}{kT}}}_{\ll 1}}$ $(\ll N_c)$

$$U = V N_c \frac{3}{2} kT F_{3/2}\left(\frac{\mu}{kT}\right) \approx \frac{3}{2} kT \underbrace{V N_c e^{\frac{E_F}{kT}}}_{\bar N\left(1 + \frac{1}{2^{3/2}}\frac{\bar N}{V N_c}\right)}\Big[1 - \frac{1}{2^{5/2}} \underbrace{e^{\frac{E_F}{kT}}}_{\frac{\bar N}{V N_c}}\Big]$$

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

$$\boxed{U \approx \frac{3}{2} kT \bar N \Big[1 + \frac{1}{2^{5/2}} \frac{\bar N}{V N_c(T)}\Big]} \quad \underline{\text{kalor. Zustandsgl.}}$$

↑ Quantenkorr. ↓

$$\boxed{pV = \frac{2}{3} U = kT \bar N \Big[1 + \frac{1}{2^{5/2}} \frac{\bar N}{V N_c(T)}\Big]} \quad \underline{\text{therm. Zustandsgl.}}$$

$$\underbrace{pv = RT}_{\text{klass. ideales Gas}}\Big(1 + \underset{\substack{\uparrow\\ \text{Fermi-Abstoßung}\\ (\underline{\text{erhöhter Druck}})}}{\frac{1}{2^{5/2}} \frac{N_A}{v N_c(T)}}\Big)$$

v Molvol.
N_A Avogadro-Konst.