

7.12.

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$$\frac{pV}{k_B T} = \sum_{\epsilon=1}^D \ln \left(1 + e^{-\beta(\epsilon - \mu)} \right)$$

Mittlere Gesamtteilchenzahl

$$\begin{aligned} N &= \frac{1}{Z_{gr}} \sum_{\alpha} N_{\alpha} e^{-\beta(\epsilon_{\alpha} - \mu N_{\alpha})} \\ &= \frac{\partial}{\partial(\beta\mu)} \ln \sum_{\alpha} e^{-\beta(\epsilon_{\alpha} - \mu N_{\alpha})} \\ &= \sum_{\ell=1}^D \frac{e^{-\beta(\epsilon_{\ell} - \mu)}}{1 + e^{-\beta(\epsilon_{\ell} - \mu)}} \\ &= \sum_{\ell=1}^D \frac{1}{e^{\beta(\epsilon_{\ell} - \mu)} + 1} = \sum_{\ell=1}^D \langle \hat{n}_{\ell} \rangle \end{aligned}$$

\hat{n}_{ℓ} Besetzungszahloperator

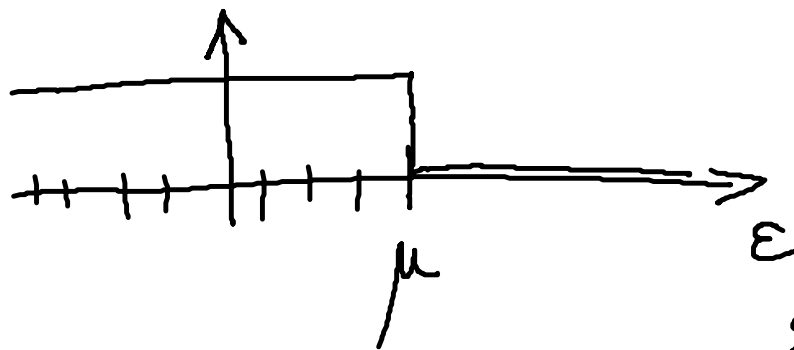
$$\langle \hat{n}_{\ell} \rangle = f(\epsilon_{\ell}) \equiv \frac{1}{e^{\beta(\epsilon_{\ell} - \mu)} + 1}$$

"Fermi-Funktion"

$$f(\epsilon) = \frac{1}{e^{\beta(\epsilon - \mu)} + 1}$$

$$\beta = \frac{1}{k_B T}$$

μ chem. Potential

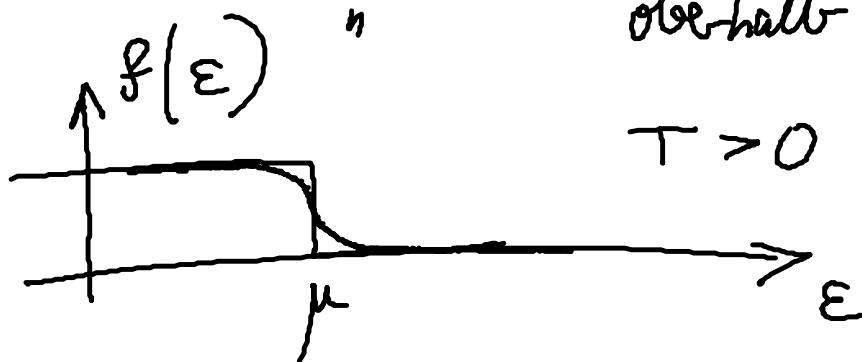


$$T=0 \Leftrightarrow \beta = \infty$$

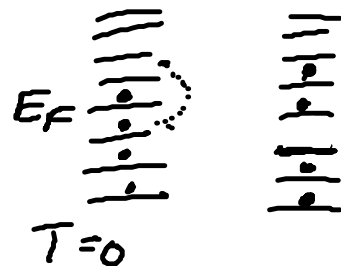
Def: $\mu(T=0) \equiv E_F$
Fermi-Energie

$$\begin{aligned} \langle n_\ell \rangle &= f(\epsilon_\ell) \stackrel{T=0}{=} \Theta(\mu - \epsilon_\ell) \\ &= \Theta(E_F - \epsilon_\ell) \end{aligned}$$

Alle 1 Teilchenzustände unterhalb E_F sind besetzt.
oberhalb E_F sind unbesetzt.



$T > 0$



Energie

$$\underline{U} = \frac{1}{Z_{gk}} \sum_{\alpha} E_{\alpha} e^{-\beta(E_{\alpha} - \mu N_{\alpha})} = \frac{D}{\ln Z_{gk}} = \frac{D}{\sum_{l=1}^D \ln(1 + e^{\beta \cdot})}$$

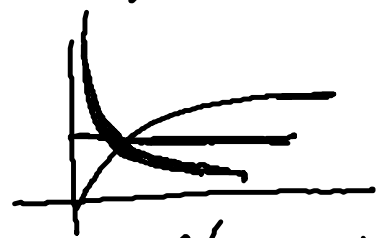
$$= \left[-\frac{\partial}{\partial \beta} + \frac{\mu}{\beta} \frac{\partial}{\partial \mu} \right] \ln Z_{gk}$$

$$= \sum_{l=1}^D \frac{\epsilon_l - \mu + \mu}{e^{\beta(\epsilon_l - \mu)} + 1} = \sum_{l=1}^D \epsilon_l f(\epsilon_l)$$

W für
Besetzung des Zustandes l

Ein teilchen zustandsdichte ν_1

$$\nu_1(\epsilon) = \sum_{l=1}^D \delta(\epsilon - \epsilon_l)$$



Damit

$$\ln Z_{gk} = \int d\epsilon \nu_1(\epsilon) \ln [1 + e^{-\beta(\epsilon - \mu)}]$$

$$U = \int d\epsilon \nu_1(\epsilon) \epsilon f(\epsilon)$$

$$N = \int d\epsilon \nu_1(\epsilon) f(\epsilon)$$

gesamte \mathcal{T} Information steckt in
der Zustandsdichte $\nu_1(\epsilon)$.

Einschub: Tricks mit der Fermi-Funktion

→ Sommerfeld-Entwicklung

1) Wir wollen Integrale des Typs

$\int d\varepsilon f(\varepsilon) g(\varepsilon)$ berechnen

$$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1}$$

Fouriertransformierte von $f(\varepsilon)$:

$$\tilde{f}(t) \equiv \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{i\omega t}}{e^{\beta(\omega-\mu)} + 1} =$$

$$= \frac{e^{i\mu t}}{2\pi i} \left[\pi i \delta(t) + \frac{1}{t} \frac{\pi t/\beta}{\sinh \pi t/\beta} \right]$$

Aufgabe

Für $T \rightarrow 0$ ist

$$\tilde{f}(t) = \frac{e^{i\mu t}}{2\pi i} \left[\pi i \delta(t) + \frac{1}{t} \right]$$

$$= \frac{e^{i\mu t}}{2\pi i} \frac{1}{t - i\delta}, \quad \delta \rightarrow 0$$

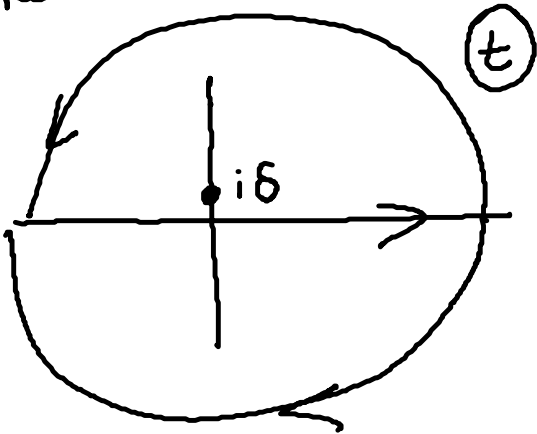
$$\lim_{\delta \rightarrow 0^+} \frac{1}{x + i\delta} = \frac{1}{x} - i\pi \delta(x)$$

Dirac-Identität (Sochozki-Plemelj-Formel)

Check: Bei $T=0$ hat man

$$f(\epsilon) = \int_{-\infty}^{\infty} \frac{dt}{2\pi i} \frac{e^{-i(\epsilon-\mu)t}}{t - i\delta}, \quad \delta \rightarrow 0^+$$

Mit Residuensatz in der komplexen t -Ebene

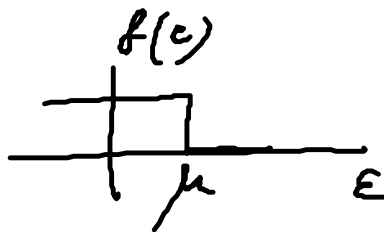


$$\epsilon - \mu < 0 \Rightarrow f(\epsilon) = 1$$

$$\epsilon - \mu > 0 \Rightarrow f(\epsilon) = 0$$

$$f(\epsilon) = \theta(\mu - \epsilon),$$

bei $T=0$!



Alternativ:

$$f(\epsilon) = \int \frac{dt}{2\pi i} \frac{e^{-i(\epsilon-\mu)t}}{t - i\delta} \stackrel{\text{Dirac}}{=}$$

$$\begin{aligned}
&= \int \frac{dt}{2\pi i} e^{-i(\varepsilon-\mu)t} \left\{ \frac{1}{t} + i\pi \delta(t) \right\} \\
&= \frac{1}{2} + \frac{1}{2\pi i} \int_{-\infty}^{\infty} dt \frac{e^{-i(\varepsilon-\mu)t}}{t} \\
&= \frac{1}{2} + \underbrace{\frac{-1}{2\pi} \int_{-\infty}^{\infty} dt \frac{\sin(\varepsilon-\mu)t}{t}}_{\pi \cdot \text{sgn}(\varepsilon-\mu)}
\end{aligned}$$

$$\varepsilon > \mu \quad : \quad 0$$

$$\varepsilon < \mu \quad : \quad 1$$

Für $T > 0$:
$$\tilde{f}(t) = \frac{e^{i\mu t}}{2\pi i} \left[\pi i \delta(t) + \frac{1}{t} \frac{\pi t/\beta}{\sinh \pi t/\beta} \right]$$

Reihenentwicklung

$$\frac{x}{\sinh x} = 1 + \sum_{n=1}^{\infty} (-1)^n \frac{2^{2n-1} B_{2n}}{(2n)!} x^{2n}$$

$$= 1 - \frac{1}{6} x^2 + \frac{7}{360} x^4 + \dots$$

B_n Bernoulli-Zahlen

\Rightarrow Sommerfeld-Entwicklung $|x| < \pi$

$$\int d\varepsilon f(\varepsilon) g(\varepsilon) = \int d\varepsilon g(\varepsilon) \int dt \tilde{f}(t) e^{-i\varepsilon t}$$

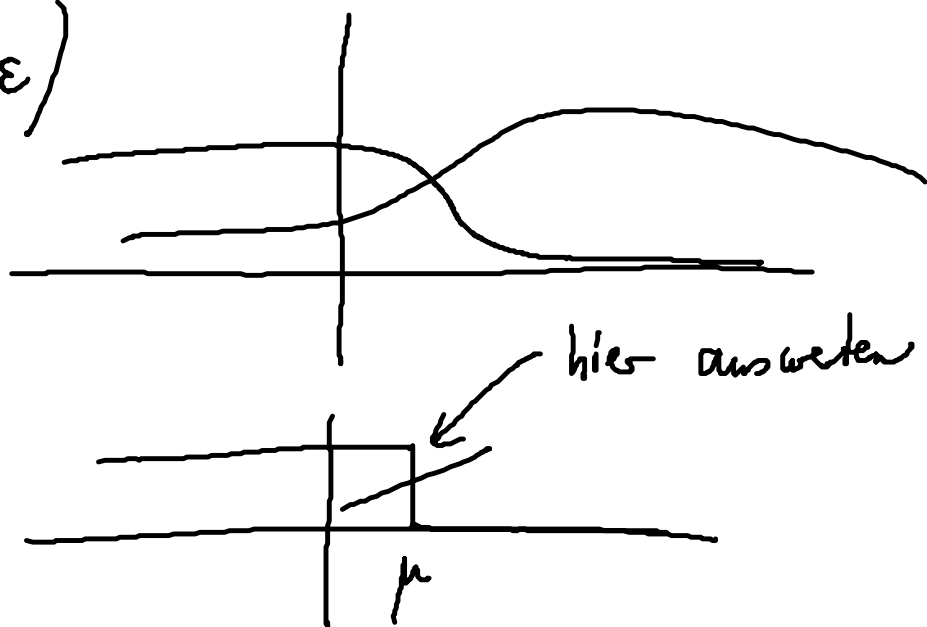
$$= \int \frac{d\varepsilon}{2\pi i} \int dt g(\varepsilon) e^{-i(\varepsilon - \mu)t} \left[\frac{1}{t - i\delta} - \frac{1}{6} \frac{\pi^2 t^2}{\beta^2} + \dots \right]$$

$$= \int d\varepsilon g(\varepsilon) \theta(\mu - \varepsilon) + \frac{\pi^2}{6} (k_B T)^2 g'(\mu) + O(T^4)$$

alles ausdrückbar durch

$$(k_B T)^{2n} g^{(n)}(\mu)$$

$$\int d\varepsilon f(\varepsilon) g(\varepsilon)$$



Die Physik spielt sich um die Fermi-Kante
 "herum ab".