7.12.

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

Mittlere Gesamtteilchenzahl

$$N = \frac{1}{Z_{gk}} \sum_\alpha N_\alpha e^{-\beta(\varepsilon_\alpha - \mu N_\alpha)}$$

$$= \frac{\partial}{\partial(\beta\mu)} \ln \sum_\alpha e^{-\beta(\varepsilon_\alpha - \mu N_\alpha)}$$

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

$$= \sum_{l=1}^{D} \frac{1}{e^{\beta(\varepsilon_l - \mu)} + 1} = \sum_{l=1}^{D} \langle \hat{n}_l \rangle$$

$\hat{n}_l$ Besetzungszahloperator

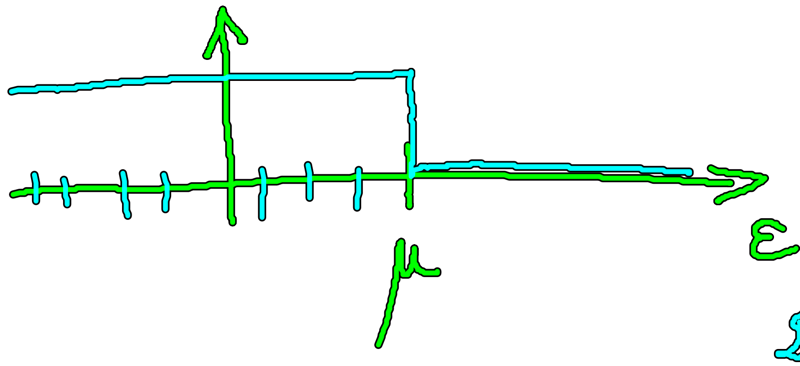
$$\langle \hat{n}_l \rangle = f(\varepsilon_l) \equiv \frac{1}{e^{\beta(\varepsilon_l - \mu)} + 1}$$

„Fermi-Funktion"

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

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

μ chem. Potential



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

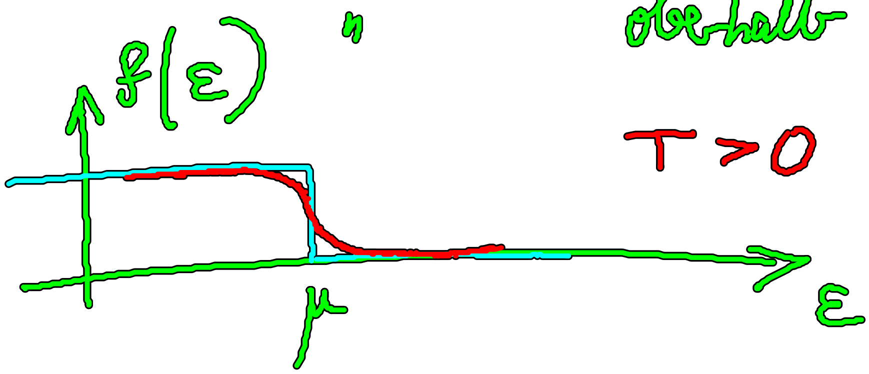
<u>Def</u>: $\mu(T=0) \equiv E_F$

Fermi-Energie

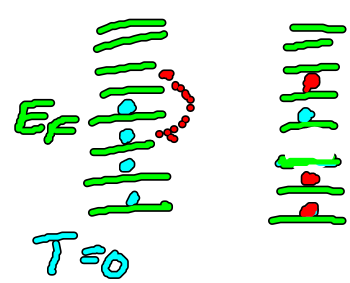
$$\langle n_\ell \rangle = f(\varepsilon_\ell) \overset{T=0}{=} \Theta(\mu - \varepsilon_\ell)$$
$$= \Theta(E_F - \varepsilon_\ell)$$

Alle 1 Teilchenzustände unterhalb E_F sind besetzt.

" oberhalb E_F sind unbesetzt.



$T>0$



Energie

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

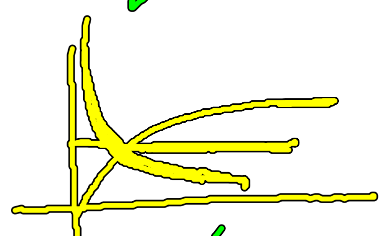
$$\ln Z_{gk} = \sum_{l=1}^{D} \ln\left(1+e^{-\beta\cdots}\right)$$

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

$$= \sum_{l=1}^{D} \frac{\varepsilon_l - \mu + \mu}{e^{\beta(\varepsilon_l - \mu)}+1} = \sum_{l=1}^{D} \varepsilon_l \underbrace{f(\varepsilon_l)}_{\text{W für Besetzung des Zustandes } l}$$

Einteilchenzustandsdichte

$$\nu_1(\varepsilon) = \sum_{l=1}^{D} \delta(\varepsilon - \varepsilon_l)$$



Damit

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

$$U = \int d\varepsilon\, \nu_1(\varepsilon)\, \varepsilon f(\varepsilon)$$

$$N = \int d\varepsilon\, \nu_1(\varepsilon) f(\varepsilon)$$

Gesamte TD Information steckt in der Zustandsdichte $\nu_1(\varepsilon)$.

Einschub: Tricks mit der Fermi-Funktion

→ Sommerfeld-Entwicklung

1) Wir wollen Integrale des Typs

$$\int d\varepsilon\, f(\varepsilon)\, g(\varepsilon) \quad \text{berechnen}$$

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

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 $T \to 0$ ist

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

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

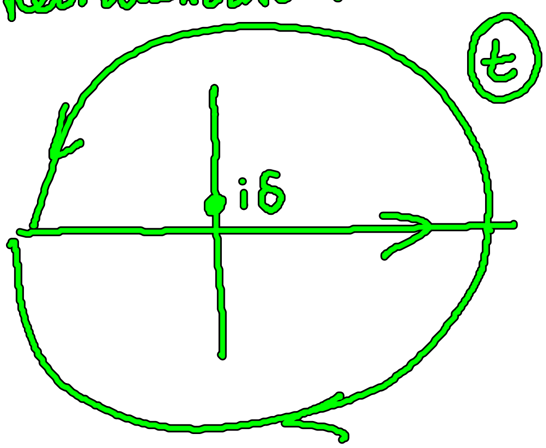
$$\lim_{\delta\to 0^+} \frac{1}{x+i\delta} = \frac{1}{x} - i\pi\,\delta(x)$$

Dirac-Identität (Sochocki-Plemelj-Formel).

Check: Bei $T=0$ hat man

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

Mit Residuensatz in der komplexen t-Ebene

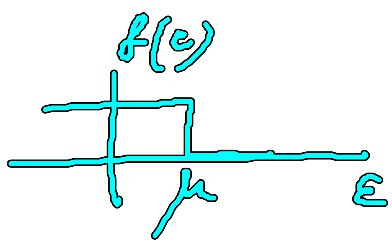


$$\varepsilon-\mu<0 \implies f(\varepsilon)=1$$

$$\varepsilon-\mu>0 \implies f(\varepsilon)=0$$

$$f(\varepsilon) = \theta(\mu-\varepsilon)$$

bei $T=0$!



$T=0$

Alternativ: $f(\varepsilon) = \int \frac{dt}{2\pi i}\, \frac{e^{-i(\varepsilon-\mu)t}}{t-i\delta} \overset{\text{Dirac}}{=}$

$$= \int \frac{dt}{2\pi i} e^{-i(\varepsilon-\mu)t} \left\{ \frac{1}{t} + i\pi\,\delta(t) \right\}$$

$$= \frac{1}{2} + \frac{1}{2\pi i} \int_{-\infty} dt \frac{e^{-i(\varepsilon-\mu)t}}{t}$$

$$= \frac{1}{2} + \frac{-1}{2\pi} \underbrace{\int_{-\infty} dt \frac{\sin(\varepsilon-\mu)t}{t}}_{\pi \cdot \operatorname{sgn}(\varepsilon-\mu)}$$

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

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

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

Reihenentwicklung?

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

B_n Bernoulli-Zahlen

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

$\Rightarrow$ Sommerfeld-Entwicklung

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

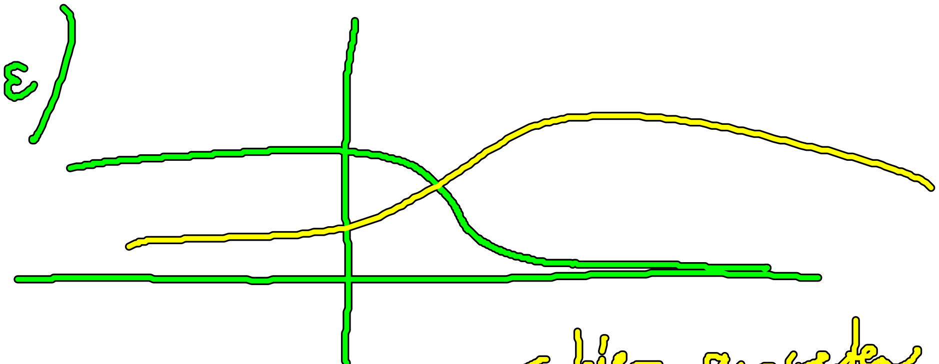
$$= \int \frac{d\varepsilon}{2\pi i} \int dt\, g(\varepsilon)\, e^{-i(\varepsilon-\mu)t} \left[\frac{1}{t-i\delta} - \frac{1}{6}\frac{\pi^2 t}{\beta^2} + \dots \right]$$

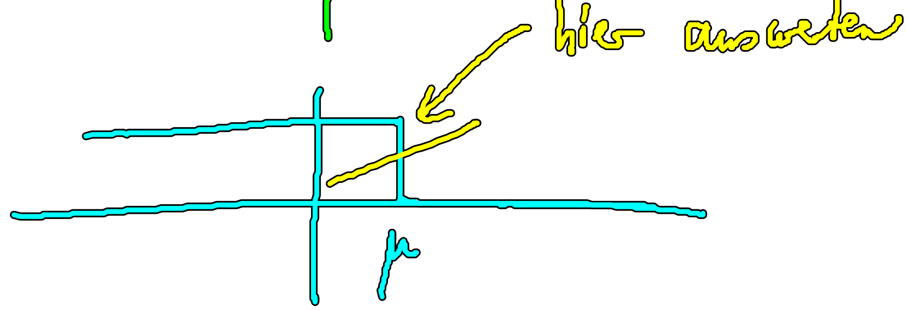
$$= \int d\varepsilon\, g(\varepsilon)\, \Theta(\mu-\varepsilon) + \frac{\pi^2}{6}(k_B T)^2\, g'(\mu) + O(T^4)$$

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".