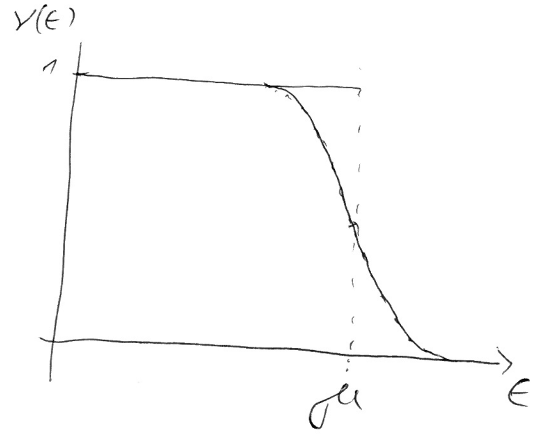
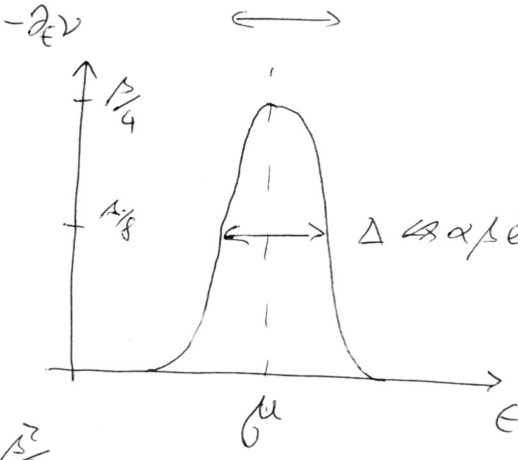
Sommerfeldův rozvoj F-D plynu při konečné teplotě (1)

- $\nu(\epsilon) = \dfrac{1}{1+e^{\beta(\epsilon-\mu)}} \xrightarrow{T=0} \begin{cases} 1 & \epsilon<\mu \\ 0 & \epsilon>\mu \end{cases}$



$\dfrac{\partial}{\partial\epsilon}$ $\longrightarrow$



$\Delta \ll \alpha\beta e^{-\frac{\beta^2}{8}} \to 0$

$$\Delta = \frac{\beta}{\cosh^2\left(\frac{\beta^2}{16}\right)} \overset{\beta\to\infty}{\propto} \frac{\beta}{e^{2\frac{\beta^2}{16}}} = \beta e^{-\frac{\beta^2}{8}}$$ $\Rightarrow$ kompaktní (β veliká)

(• $\Omega = -k_B T \int_0^\infty d\epsilon\, D(\epsilon) \log(1+e^{-\beta(\epsilon-\mu)}) = -\int_0^\infty d\epsilon\, \Gamma(\epsilon)\nu(\epsilon)$ … $\Gamma(\epsilon)=\int_0^\epsilon D(\epsilon')d\epsilon'$

$D(\epsilon) \propto \epsilon^\alpha$ … hust. stavů)

- $\boxed{\langle A\rangle = \int d\epsilon\, A(\epsilon) D(\epsilon)\nu(\epsilon)}$

$\Rightarrow$ potřebujeme integrály $I(T) = \int d\epsilon\, G(\epsilon)\nu(\epsilon)$

$G(\epsilon)$: a) $\to 0$ $\quad \epsilon\to-\infty$ (∃ práh)

b) $\propto \epsilon^\alpha$ $\quad \epsilon\to+\infty$

c) $\in C(\mathcal{U}(\mu))$

- per partes:

$$I(T) = \nu(\epsilon)\underbrace{\int_{-\infty}^{\epsilon} G(\epsilon')d\epsilon'}_{J(\epsilon)}\Bigg|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} d\epsilon\, J(\epsilon)\,\partial_\epsilon\nu(\epsilon)$$

$$J(\epsilon) = \int_{-\infty}^{\epsilon} G(\epsilon')d\epsilon \begin{cases} \propto \epsilon^{\gamma} & \epsilon\to\infty \Rightarrow \times\nu(\epsilon)\to 0 \\ \to 0 & \epsilon\to-\infty \Rightarrow \times\nu(\epsilon)\to 0 \end{cases}$$

$$\Rightarrow I(T) = -\int_{-\infty}^{\infty} J(\epsilon)\, \partial_\epsilon \nu(\epsilon)\, d\epsilon$$

$J(\epsilon)$
- $\in C^1$
- $\propto \epsilon^{\gamma}$ ~~a~~ $\epsilon \to \infty$
- $\to 0$ $\quad \epsilon \to -\infty$

- Rozvoj J – díky kompaktnosti $\frac{\partial \nu(\epsilon)}{\partial \epsilon}$ nás $J(\epsilon)$ zajímá jen okolo μ

$$J(\epsilon) = J(\mu) + \sum_{n=1}^{\infty} \frac{1}{n!} (\epsilon-\mu)^n\, \partial_\epsilon^n J(\epsilon)\big|_{\epsilon=\mu}$$

- $\partial_\epsilon \nu(\epsilon) = -\dfrac{\beta}{4\cosh\left(\frac{\beta}{2}(\epsilon-\mu)\right)}$ je sudá kolem μ $\Rightarrow$ pouze sudé členy v rozvoji $J(\epsilon)$ přispějí

$\dfrac{\beta e^{\beta(\epsilon-\mu)}}{(1+e^{\beta()})^2}$

$$\Rightarrow I(T) = -J(\mu) \underbrace{\int_{-\infty}^{\infty} \cancel{\nu(\epsilon)}\, \partial_\epsilon \nu(\epsilon)\, d\epsilon}_{\nu(+\infty)-\nu(-\infty) = -1} - \sum_{n=1}^{\infty} \frac{1}{(2n)!} \partial_\epsilon^{2n} J(\epsilon)\big|_\mu \int_{-\infty}^{\infty} d\epsilon\, (\epsilon-\mu)^{2n}\, \partial_\epsilon \nu(\epsilon)$$

$$\Rightarrow \boxed{I(T) = J(\mu) + \sum_{n=1}^{\infty} \frac{1}{(2n)!} \partial_\epsilon^{2n} J(\epsilon)\big|_\mu \int_{-\infty}^{\infty} d\epsilon\, (\epsilon-\mu)^{2n} \frac{\beta e^{\beta(\epsilon-\mu)}}{(1+e^{\beta(\epsilon-\mu)})^2}}$$

- obecně lze ještě provést integraci $\Rightarrow$ vyjádření pomocí Riemanovy ζ fce (viz studijní text, samozřejmě v jiném značení)

$\boxed{n=1}$

- $\displaystyle\int_{-\infty}^{\infty} = \Big/ \begin{matrix} \beta(\epsilon-\mu) = x \\ \beta d\epsilon = dx \end{matrix} \Big/ = \frac{2}{\beta^2} \int_0^{\infty} dx \frac{x^2 e^x}{(1+e^x)^2} = \frac{2}{\beta}\Big[\underbrace{-x^2(1+e^x)^{-1}}_{\to 0}\Big]_0^{\infty}$

$$+\frac{2}{\beta^2}\int_0^{\infty} \frac{2x}{1+e^x}\, dx \overset{\text{polylog? - řadou?}}{=} \frac{\pi^2}{3\beta^2} = \frac{\pi^2}{3}(k_B T)^2$$

Je to Rieman. $\zeta(2)$ fce

$$\boxed{\int \frac{x}{1+e^x}\, dx = \frac{\pi^2}{12}}$$

$$\partial_\epsilon J(\epsilon) = G(\epsilon) \to \partial_\epsilon^2 J(\epsilon)\big|_\mu = G'(\mu)$$

$$\Rightarrow \boxed{I(T) = J(\mu) + \frac{\pi^2}{6}(k_B T)^2 G'(\mu)}$$

$G(\epsilon) = A(\epsilon) D(\epsilon)$

$J(\epsilon) = \int^{\epsilon} G(\epsilon')\, d\epsilon'$

Oprava k chem. potenciálu

počítejme $\langle N \rangle$ $\Leftrightarrow$ $A(\epsilon)=1$

$$\Rightarrow \langle N \rangle_{(\mu,T)} = \underbrace{\int_{-\infty}^{\mu} D(\epsilon)\,d\epsilon}_{J(\mu)=\int_{-\infty}^{\mu} G(\epsilon)d\epsilon} + \frac{\pi^2}{6}(k_B T)^2 D'(\mu)$$

$$\Big\downarrow \text{ inverze}$$

$$\mu(N,T)$$

NB: fyz. interpretace Sommerfelda:

malé $k_B T$ $\rightarrow$ přeskoky možné jen mezi energeticky blízkými 1p stavy – ty jsou k dispozici jen v malém okolí ~~Fe~~ Fermiho meze (obsaz. těsně pod $\rightarrow$ neobsaz. těsně nad)

$\rightarrow$ spec. koefs lin. odezvy závisí pouze na vlastnostech (ie, hustotě stavů) systému v okolí ~~Fe~~ Fermiho meze

Id. plyn:

$$D(\epsilon) = \frac{4\pi V}{h^3}(2m)^{3/2}\epsilon^{1/2} \Rightarrow D'(\epsilon) = \frac{2\pi V}{h^3}(2m)^{3/2}\epsilon^{-1/2}$$

$$\Rightarrow \Gamma(\epsilon) = \frac{8\pi V}{3h^3}(2m)^{3/2}\epsilon^{3/2}$$

$$\Rightarrow \frac{N}{V} = \frac{8\pi}{3h^3}(2m)^{3/2}\mu^{3/2} + \frac{\pi^2}{6}(k_B T)^2 \frac{2\pi}{h^3}(2m)^{3/2}\mu^{-1/2} \cdot$$

$$\times \frac{8\epsilon_F^{3/2}}{8\epsilon_F^{3/2}}$$

$$n = \frac{8\pi}{3h^3}(2m)^{3/2}\epsilon_F^{3/2}$$

$$\Rightarrow n = n\left(\frac{\mu}{\epsilon_F}\right)^{3/2} + \frac{\pi^2}{8}(k_B T)^2 n \frac{\mu^{-1/2}}{\epsilon_F^{3/2}}$$

$$= n\left(\frac{\mu}{\epsilon_F}\right)^{3/2}\left(1 + \frac{\pi^2}{8}(k_B T)^2 \mu^{-2}\right)$$

$$\Rightarrow 1 = \left(\frac{\mu}{\epsilon_F}\right)^{3/2}\left[1+\frac{\pi^2}{8}\left(\frac{k_B T}{\epsilon_F}\right)^2\left(\frac{\epsilon_F}{\mu}\right)^2\right]$$

(nemohu počítat dál než do T^2 (resp. T^3, ale to tam není)

$$\mu = \epsilon_F + \alpha T^2 \Rightarrow$$ zde přispěje jen 1, αT^2 už vede na T^4

$$\Rightarrow \left(\frac{\epsilon_F}{\mu}\right)^{3/2} = 1 + \frac{\pi^2}{8}\left(\frac{k_B T}{\epsilon_F}\right)^2$$

$$\Rightarrow \frac{\mu}{\epsilon_F} = \left[1+\frac{\pi^2}{8}\left(\frac{k_B T}{\epsilon_F}\right)^2\right]^{-2/3} \Rightarrow \boxed{\frac{\mu}{\epsilon_F} = 1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\epsilon_F}\right)^2}$$

$$\cancel{1 = x^{3/2}(1 + \alpha T^2 x^2)}$$

$$1 = x^{3/2}(1+\alpha T^2 x^{-2}) \qquad x = 1 + \lambda_1 T + \lambda_2 T^2 \ldots$$

$$1 = (1+\lambda_1 T + \lambda_2 T^2)^{3/2}\left[1 + \alpha T^2 (1+\lambda_1 T + \lambda_2 T^2)^{-2}\right]$$

$$(1+\alpha T^2(1+\lambda_1 T + \lambda_2 T^2)^{-2})^{-1} = (1+\lambda_1 T + \lambda_2 T^2)^{3/2}$$

$$(1+\alpha T^2(1-2(\lambda_1 T + \lambda_2 T^2)))^{-1} = 1 + \frac{3}{2}(\lambda_1 T + \lambda_2 T^2)$$

$$= 1 - \alpha T^2(1 - 2\lambda_1 T - 2\lambda_2 T^2) = 1 + \frac{3}{2}(\lambda_1 T + \lambda_2 T^2)$$

řád T^0: $1 = 1$

T^1: $0 = \lambda_1$

T^2: $-\alpha = \frac{3}{2}\lambda_2 \Rightarrow \alpha = \frac{\pi^2}{8}\left(\frac{k_B}{\epsilon_F}\right)^2 = -\frac{3}{2}\lambda_2$

$$\Rightarrow \lambda_2 = -\frac{\pi^2}{12}\left(\frac{k_B}{\epsilon_F}\right)^2 \Rightarrow \text{OK!}$$

Pauliho paramagnet: – částice se spinem v mg. poli ⇒ χ? (1)

$$\boxed{\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 - \hat{\vec{M}}\cdot\hat{\vec{H}} = \sum_{\vec{k},\sigma}\left(\vec{\epsilon}_k - g\mu_B\sigma H_z\right)\hat{c}^{+}_{\vec{k}\sigma} c_{\vec{k}\sigma}}$$

$$\vec{\mu} = g\mu_B\vec{\sigma} \qquad \mu_B = \frac{e\hbar}{2m} \qquad \sigma = \pm\tfrac{1}{2}$$

$\{dU = TdS + MdM$ – paramagnetika$\}$

$$\Rightarrow \Omega = -\frac{1}{\beta}\sum_\sigma \int d\epsilon\, D_\sigma(\epsilon)\log\left[1 + e^{-\beta(\epsilon - g\mu_B\sigma H_z - \mu)}\right]$$

$[d\Omega = -SdT - MdH]$ ... paramagnetika

$$\Rightarrow \langle M_z\rangle = -\frac{\partial\Omega}{\partial H_z} = \frac{1}{\beta}\sum_\sigma\int d\epsilon\, D_\sigma(\epsilon)\frac{e^{-\beta(\epsilon - g\mu_B\sigma H_z - \mu)}}{1+e^{-\beta(\epsilon - g\mu_B H_z - \mu)}} \times$$

$$\times\, \beta g\mu_B\sigma$$

$$\Rightarrow \langle M_z\rangle = g\mu_B\sum_\sigma\sigma\underbrace{\int d\epsilon\, D_\sigma(\epsilon)\, \nu(\epsilon - g\mu_B\sigma H)}_{N_\sigma}$$

$$\Rightarrow \langle M_z\rangle = \frac{1}{2}g\mu_B\left(N_\uparrow - N_\downarrow\right)$$

Slabé pole (lin. odezva)

- $\nu(\epsilon - g\mu_B\sigma H) = \nu(\epsilon) - g\mu_B\sigma H\,\partial_\epsilon\nu$
- $D_\uparrow(\epsilon) = D_\downarrow(\epsilon) = \frac{1}{2}D(\epsilon)$

$$\Rightarrow \langle M_z\rangle = -(g\mu_B)^2 H\,(\overset{1/4}{\overbrace{2\sigma^2}})\int d\epsilon\,\frac{1}{2}D(\epsilon)\,\partial_\epsilon\nu$$

$$= -(g\mu_B)^2 H\,\frac{1}{4}\int d\epsilon\, D(\epsilon)\,\partial_\epsilon\nu \quad = /g=2/$$

$$\Rightarrow \langle M_z\rangle = -\mu_B^2 H\int d\epsilon\, D(\epsilon)\,\partial_\epsilon\nu$$

(2)

$\Rightarrow$ Srov. Sommerfeld

$$I(T) = -\int_{-\infty}^{\infty} d\epsilon\, J(\epsilon)\, \partial_\epsilon \nu \approx J(\mu) + \frac{\pi^2}{6}(k_B T)^2 J''(\mu)$$

Zde $J(\epsilon) = \mu_B^2 H D(\epsilon)$

$$\Rightarrow \langle M \rangle = \mu_B^2 H D(\mu) + \frac{\pi^2}{6}(k_B T)^2 \mu_B^2 H \left.\frac{d^2 D(\epsilon)}{d\epsilon^2}\right|_\mu$$

Dále to umíme pro id. plyn:

$$D(\epsilon) = \frac{4\pi V}{h^3}(2m)^{3/2}\epsilon^{1/2} \Rightarrow D'(\epsilon) = \frac{D(\epsilon)}{2\epsilon}$$

$$\Rightarrow D''(\epsilon) - \frac{D(\epsilon)}{4\epsilon^2}$$

$$\Rightarrow \chi_T = \left(\frac{\partial M}{\partial H}\right)_T = \mu_B^2 D(\mu)\left[1 - \frac{\pi^2}{24}\left(\frac{k_B T}{\mu}\right)^2\right]$$

$$\frac{\mu}{\epsilon_F} = 1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\epsilon_F}\right)^2 + o(T^2)$$

$$\Rightarrow \frac{D(\mu)}{D(\epsilon_F)} = \left(\frac{\mu}{\epsilon_F}\right)^{1/2} = 1 - \frac{\pi^2}{24}\left(\frac{k_B T}{\epsilon_F}\right)^2 + o(T^2)$$

$$\Rightarrow \chi_T = \mu_B^2 D(\epsilon_F)\frac{D(\mu)}{D(\epsilon_F)}\left[1 - \frac{\pi^2}{24}\left(\frac{k_B T}{\epsilon_F}\right)^2\left(\frac{\epsilon_F}{\mu}\right)^2\right]$$

$$= \mu_B^2 D(\epsilon_F)\left[1 - \frac{\pi^2}{24}\left(\frac{k_B T}{\epsilon_F}\right)^2\right]\left[1 - \frac{\pi^2}{24}\left(\frac{k_B T}{\epsilon_F}\right)^2\left(1 + \cancel{\frac{\pi^2}{12}\left(\frac{k_B T}{\epsilon_F}\right)^2}\right)\right]$$

$$= \mu_B^2 D(\epsilon_F)\left[1 - \frac{\pi^2}{24}\left(\frac{k_B T}{\epsilon_F}\right)^2 - \frac{\pi^2}{24}\left(\frac{k_B T}{\epsilon_F}\right)^2\right]$$

$$N = \Gamma(\epsilon_F) = \frac{2}{3}D(\epsilon_F)\epsilon_F \Rightarrow \boxed{\chi_T = \frac{3N}{2\epsilon_F}\mu_B^2\left(1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\epsilon_F}\right)^2\right)}$$