- pressure of Bose-Einstein gas lower than classical pressure since particles in ground state do not contribute to pressure
- pressure of Fermi-Dirac gas higher than classical pressure since no state can have more than one particle → low momentum states have less particles than classically → high momentum states have more particles than classically

$\downarrow 3/2$

$\downarrow 3/4$

Low temperature thermodynamics

Given N and V what is μ'?

$$N = \int_{-\infty}^{\infty} n(\varepsilon)\, \frac{g}{e^{\beta(\varepsilon-\mu')}+1}\, d\varepsilon$$

$n(\varepsilon)$: density of states

$\Omega(\varepsilon)$ = # of states below energy ε

$n(\varepsilon) = \frac{d}{d\varepsilon}\Omega(\varepsilon)$

$\Omega(\varepsilon)$ = # of $\vec{l}$ with $\frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 \vec{l}^{\,2} \leq \varepsilon$

$$\Rightarrow \Omega(\varepsilon) = \frac{4}{3}\pi \left(\frac{2m\varepsilon}{h^2}\right)^{3/2} V$$

$$\Rightarrow n(\varepsilon) = \begin{cases} 2\pi V \left(\frac{2m}{h^2}\right)^{3/2} \varepsilon^{1/2} & \varepsilon > 0 \\ 0 & \varepsilon < 0 \end{cases}$$

at $T=0$: $\mu' = \varepsilon_F$ $\quad \frac{g}{e^{\beta(\varepsilon-\mu')}+1} = \begin{cases} g & \varepsilon < \varepsilon_F \\ 0 & \varepsilon > \varepsilon_F \end{cases}$

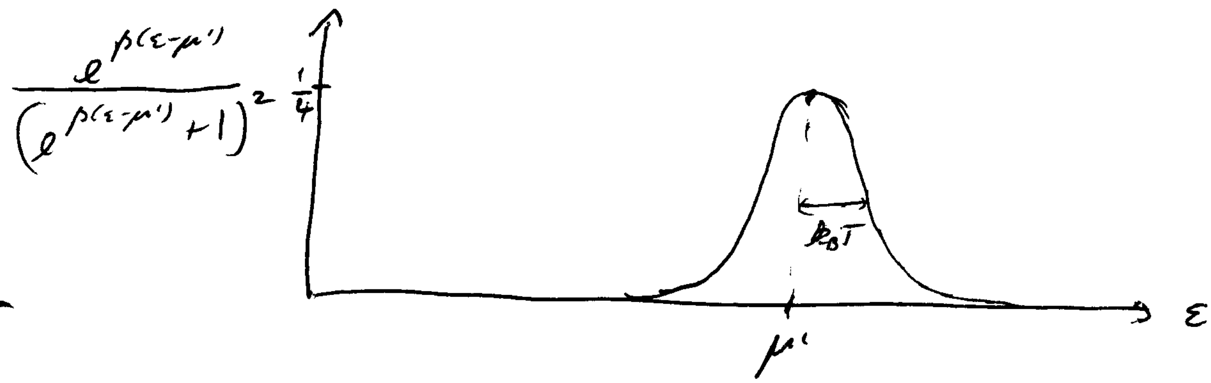
$$N = \int_{-\infty}^{\varepsilon_F} n(\varepsilon)\, g\, d\varepsilon = g\,\Omega(\varepsilon_F) = \frac{4}{3}\pi g \left(\frac{2m\varepsilon_F}{\hbar^2}\right)^{3/2} V$$

$$\Rightarrow \varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{6\pi^2 n}{g}\right)^{2/3} \qquad \Rightarrow \Omega(\varepsilon) = \frac{N}{g}\left(\frac{\varepsilon}{\varepsilon_F}\right)^{3/2}$$

$$n(\varepsilon) = \frac{3N}{2g}\,\frac{\varepsilon^{1/2}}{\varepsilon_F^{3/2}}$$

at $T \simeq 0$

$$N = \int_{-\infty}^{\infty} n(\varepsilon)\,\frac{g}{e^{\beta(\varepsilon-\mu')}+1}\,d\varepsilon \overset{PI}{=} \int_{-\infty}^{\infty} \Omega(\varepsilon)\,\frac{g\beta e^{\beta(\varepsilon-\mu')}}{\left(e^{\beta(\varepsilon-\mu')}+1\right)^2}\,d\varepsilon$$



"all physics in a Fermi-Dirac gas close to $T=0$ happens in an energy range of k_BT around the chemical potential $\mu' \simeq \varepsilon_F$"

$$N = g\int_{-\infty}^{\infty} \Omega(t k_BT + \mu')\,\frac{e^t}{(e^t+1)^2}\,dt$$

$$= g\int_{-\infty}^{\infty} \Omega(\mu')\,\frac{e^t}{(e^t+1)^2}\,dt + g\,\Omega'(\mu')\,k_BT\int_{-\infty}^{\infty} t\,\frac{e^t}{(e^t+1)^2}\,dt$$

$$+ g\left(\frac{d^2\Omega}{d\varepsilon^2}(\mu')\right)\frac{(k_BT)^2}{2}\int_{-\infty}^{\infty} t^2\,\frac{e^t}{(e^t+1)^2}\,dt + O\left((k_BT)^3\right)$$

need $I_n = \int_{-\infty}^{\infty} t^n \frac{e^t}{(e^t+1)^2} dt$

$I_n = 0$ for n odd $\quad I_0 = 1 \quad I_2 = \frac{\pi^2}{3}$, $I_4 = \frac{7\pi^4}{15}$

$$N = g \frac{N}{g} \left(\frac{\mu'}{\varepsilon_F}\right)^{3/2} + g \frac{(k_B T)^2}{2} \frac{N}{g\,\varepsilon_F^{3/2}} \frac{3}{4} \mu'^{-1/2} \frac{\pi^2}{3} + O((k_B T)^4)$$

$\mu' = \varepsilon_F (1 + \delta\mu')$

$$N = N(1+\delta\mu')^{3/2} + N \frac{(k_B T)^2 \pi^2}{8\, \varepsilon_F^{2}} (1+\delta\mu')^{-1/2} + O((k_B T)^4)$$

$$N = N + \frac{3}{2} N \delta\mu' + N \frac{(k_B T)^2}{8} \frac{\pi^2}{\varepsilon_F^{2}} + O((k_B T)^4)$$

$$\Rightarrow \delta\mu' = -\frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F}\right)^2 \Rightarrow \mu' = \varepsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F}\right)^2 + O((k_B T)^4)\right]$$

<u>internal energy</u>

$$U = \int_{-\infty}^{\infty} d\varepsilon \; n(\varepsilon)\, \varepsilon \frac{g}{e^{\beta(\varepsilon-\mu')}+1}$$

at $T=0$ $\quad U = \int_0^{\varepsilon_F} d\varepsilon \; \varepsilon\, n(\varepsilon) g = \frac{Ng}{g\,\varepsilon_F^{3/2}} \frac{3}{2} \int_0^{\varepsilon_F} d\varepsilon \; \varepsilon^{3/2} = \frac{3}{5} N \varepsilon_F$

at $T \neq 0$: $\quad U = \frac{3N}{2g\,\varepsilon_F^{3/2}} \int_{-\infty}^{\infty} d\varepsilon \; \varepsilon^{3/2} \frac{g}{e^{\beta(\varepsilon-\mu')}+1}$

$$= \frac{3N}{5\,\varepsilon_F^{3/2}} \int_{-\infty}^{\infty} d\varepsilon \; \varepsilon^{5/2} \frac{\beta e^{\beta(\varepsilon-\mu')}}{(e^{\beta(\varepsilon-\mu')}+1)^2}$$

$$= \frac{3N}{5\,\varepsilon_F^{3/2}} \int_{-\infty}^{\infty} dt \; (k_B T t + \mu')^{5/2} \frac{e^t}{(e^t+1)^2}$$

$$= \frac{3N}{5\varepsilon_F^{3/2}} \mu^{5/2} + \frac{3N}{5\varepsilon_F^{3/2}} \frac{1}{2}(k_B T)^2 \cdot \frac{15}{4} \mu^{1/2} \underbrace{I_2}_{\frac{\pi^2}{3}} + O((k_B T)^4)$$

$$= \frac{3N}{5} \varepsilon_F \left(1 - \frac{5}{2}\frac{\pi^2}{12}\left(\frac{k_B T}{\varepsilon_F}\right)^2\right) + \frac{3}{8} N \varepsilon_F \left(\frac{k_B T}{\varepsilon_F}\right)^2 \pi^2 + O((k_B T)^4)$$

$$= \frac{3N}{5} \varepsilon_F \left[1 + \frac{5}{12}\pi^2 \left(\frac{k_B T}{\varepsilon_F}\right)^2 + O((k_B T)^4)\right]$$

$$\Rightarrow C_V = \left(\frac{\partial U}{\partial T}\right)_{V, \{N\}} = \frac{N\pi^2}{2\varepsilon_F} k_B^2 T \quad \sim T$$

<u>High temperatures:</u>

$$0 \leftarrow \frac{n\lambda_T^3}{g} = f_{3/2}(z) \quad \Rightarrow \quad z \to 0 \quad \Rightarrow \quad f_{3/2}(z) \simeq z$$

$$\Rightarrow z \approx \frac{n\lambda_T^3}{g}$$

$$P = \frac{k_B T g}{\lambda_T^3} f_{5/2}(z) \simeq \frac{k_B T g}{\lambda_T^3} f_{5/2}\left(\frac{n\lambda_T^3}{g}\right) \simeq \frac{k_B T g}{\lambda_T^3} \frac{n\lambda_T^3}{g}$$

$$= n k_B T = \frac{N k_B T}{V}$$

back to the ideal gas

VI 6 Summary

concepts:

density operator
pure state / mixed state
ideal Bose-Einstein gas
quantum-mechanical size of a particle
ideal Fermi-Dirac gas
Fermi sea, Fermi energy, Fermi momentum, Fermi temperature

facts:

time evolution of a density operator
calculating probabilities from a density operator
density operators of thermodynamic ensembles
basis of 2- and 3-particle Hilbert space and Fock-space
pressure increased for fermions / decreased for bosons
Bose-Einstein condensation
expected number of particles per state in Bose-Einstein
and Fermi-Dirac gas

tools:

calculating exponentials of matrices
extremization in operator space
expansion around ε_F in Fermi-Dirac gas

VII Numerical methods

- ~~F~~or most microscopic models neither $N(E)$, nor $Z(T)$, nor $Z(T,\mu')$ can be calculated
- still want to know macroscopic behavior of microscopic models

$\Rightarrow$ numerical studies

VII.1 Monte Carlo simulation

VII.1.1 General concept

States $i = 1, \dots, N$, energies E_i
Want to know (or estimate) π_i.

"Invent" dynamics (this is not the real dynamics)
$w_{i\to j}$ = probability that system jumps from state i to state j from t to $t+1$ given that it is in state i

Ensemble of M systems, $n_i(t)$ # systems in state i at time t

$$n_i(t+1) = n_i(t) - \sum_{\substack{j=1\\ j\neq i}}^{N} w_{i\to j}\, n_i(t) + \sum_{\substack{j=1\\ j\neq i}}^{N} w_{j\to i}\, n_j(t)$$

"Master equation"
We are interested in stationary state

$\Rightarrow n_i(t+1) = n_i(t)$

$$\Rightarrow \sum_{\substack{j=1 \\ j\neq i}}^{N} [w_{j\to i}\, n_j - w_{i\to j}\, n_i] = 0$$

Can make sure that this holds by choosing $w_{j\to i}$ such that

$$w_{j\to i}\, n_j = w_{i\to j}\, n_i \quad \text{for all } i \text{ and } j$$

"detailed balance"

$$w_{j\to i} = w_{i\to j}\,\frac{n_i}{n_j} = w_{i\to j}\,\frac{\rho_i}{\rho_j} = w_{i\to j}\, e^{-\beta(E_i - E_j)}$$

do not need to know partition function $Z(T)$ ☺

3/4
3/11

In practice:

- Choose most $w_{i\to j}$ to be zero as long as
  - if $w_{i\to j}=0$ then also $w_{j\to i}=0$
  - it is possible for the system to go from any i to any j through intermediate states
- Choose $w_{i\to j} = \begin{cases} 1 & E_j \leq E_i \\ e^{-\beta(E_j - E_i)} & E_i < E_j \end{cases}$ *
- Look at time evolution of a single system instead of an ensemble