quatum effects introduce an effective "interaction" between particles. In the last chapter (about interacting particles, we learned that

$$\ln Z = \ln Z_0 + \frac{N^2}{2V} \int d^3\vec{r} \left(e^{-\beta U(\vec{r})} - 1 \right) + \dots$$

Thus the "effective potential" due to quantum effect is

$$U(\vec{r}) = -k_B T \ln\left(1 + \eta e^{-2\pi r^2/\lambda^2}\right) \simeq -k_B T \eta e^{-2\pi r^2/\lambda^2}$$

this is a Gausian form with <u>range</u> of interaction equal λ – the thermal length!

$\boxed{\text{Grand canonical formulation}}$

Calculating Z_N with all possible permutations is a formidable task. It's much easier to use grand canonical formulation and energy basis.

$$Z_N = \mathrm{Tr}\left[\exp(-\beta \hat{H})\right] = \sum_{\{\vec{k}\}}{}' \exp\left[-\beta \sum_{i=1}^{N} \varepsilon_{\vec{k}_i}\right]$$

$$= \underbrace{\sum_{\{n_{\vec{k}}\}}{}'}_{\text{sum is restricted to } \sum_{\vec{k}} n_{\vec{k}} = N} \exp\left[-\beta \sum_{\vec{k}} \varepsilon_{\vec{k}} n_{\vec{k}}\right]$$

. This restriction can be remove by looking at grand canonical partition function

$$\mathcal{Z} = \sum_{N=0}^{\infty} e^{\beta\mu N} Z_N = \sum_{\{n_k\}} \exp\left[-\beta \sum_{\vec{k}} (\varepsilon_{\vec{k}} - \mu) n_{\vec{k}}\right]$$

$$= \sum_{\{n_k\}} \prod_{\vec{k}} \exp\left[-\beta(\varepsilon_{\vec{k}}-\mu)\, n_{\vec{k}}\right]$$

$$= \prod_{\vec{k}} \left\{ \sum_{\{n_k\}} \exp\left(-\beta(\varepsilon_{\vec{k}}-\mu)\, n_{\vec{k}}\right) \right\}$$

For Fermions, n_k can have only 2 values 0 and 1. So the term in the $\{\ \}$ is $1+\exp\left[-\beta(\varepsilon_k-\mu)\right]$

and $$\mathcal{Z}^- = \prod_{\vec{k}} \left(1+\exp\left[-\beta(\varepsilon_k-\mu)\right]\right)$$

For Bosons, $n_k = 0, 1, 2, \ldots$ so the term inside $\{\ \}$ is

$$\left\{1-\exp\left[-\beta(\varepsilon_{\vec{k}}-\mu)\right]\right\}^{-1}$$ and

$$\mathcal{Z}^+ = \prod_{\vec{k}} \left(1-\exp\left[-\beta(\varepsilon_{\vec{k}}-\mu)\right]\right)^{-1}$$

We can write for both cases:

$$\boxed{\ln \mathcal{Z}^\eta = -\eta \sum_{\vec{k}} \ln\left\{1-\eta\exp\left[-\beta(\varepsilon_k-\mu)\right]\right\}}$$

again $\eta = +1$ for bosons $\eta = -1$ for Fermions.

one can use the set $\{n_{\vec{k}}\}$ to specify one quantum microstate.

In grand canonical ensemble, the probability for a microstate is

$$P_\eta(\{n_{\vec{k}}\}) = \frac{1}{\mathcal{Z}^\eta} \cdot \prod_{\vec{k}} \exp\left[-\beta(\varepsilon_{\vec{k}}-\mu)\, n_{\vec{k}}\right]$$

The average occupation number $n_{\vec{k}}$ for a particular one-particle state $|\vec{k}\rangle$ is then

$$\langle n_{\vec{k}} \rangle_\eta = \sum_{\{n_{\vec{k}'}\}} n_{\vec{k}}\, P_\eta(\{n_{\vec{k}'}\})$$

$$= -\frac{1}{\mathcal{Z}^\eta} \cdot \frac{\partial \mathcal{Z}^\eta}{\partial(\beta \varepsilon_{\vec{k}})} = -\frac{\partial \ln \mathcal{Z}^\eta}{\partial(\beta \varepsilon_{\vec{k}})}$$

$$= \frac{\partial}{\partial(\beta \varepsilon_{\vec{k}})} \cdot \left\{ -\eta \ln \left(1 - \eta \exp\left[-\beta(\varepsilon_{\vec{k}} - \mu)\right]\right) \right\}$$

$$\boxed{\langle n_{\vec{k}} \rangle_\eta = \frac{1}{z^{-1} e^{\beta \varepsilon_{\vec{k}}} - \eta}} \qquad z = e^{\beta\mu} \text{ - fugacity}$$

Since this is an important result, we write explicitly the occupation number for bosons:

$$\langle n_{\vec{k}} \rangle_+ = \frac{1}{e^{\beta(\varepsilon_{\vec{k}} - \mu)} - 1}$$

and fermions

$$\langle n_k \rangle_- = \frac{1}{e^{\beta(\varepsilon_k - \mu)} + 1} \leq 1 .$$

The average number of particles in grand canonical is

$$N_\eta = \sum_{\vec{k}} \langle n_{\vec{k}} \rangle_\eta = \sum_{\vec{k}} \frac{1}{e^{\beta(\varepsilon_{\vec{k}} - \mu)} - \eta}$$

The average energy is grand canonical is

$$E_\eta = \sum_{\vec{k}} \varepsilon_{\vec{k}} \langle n_{\vec{k}} \rangle_\eta = \sum_{\vec{k}} \frac{\varepsilon_{\vec{k}}}{e^{\beta(\varepsilon_{\vec{k}} - \mu)} - \eta}$$

Note that quantum particles are oftenly characterized further by spin s. In this case the degeneracy factor $g = 2s+1$ has to multiply the above formulae when there's no external magnetic field

$$N_\eta = g \sum_{\vec{k}} \frac{1}{z^{-1} e^{\beta \varepsilon_k} - \eta}, \quad E_\eta = g \sum_{\vec{k}} \frac{\varepsilon_k}{z^{-1} e^{\beta \varepsilon_k} - \eta}$$

And the high T virial expansion

$$P_\eta = n_\eta kT \left[1 - \frac{\eta}{2^{5/2}} \left(\frac{n_\eta \lambda^3}{g} \right) + \left(\frac{1}{8} - \frac{2}{3^{5/2}} \right) \left(\frac{n_\eta \lambda^3}{g} \right)^2 + \dots \right]$$

For low T, Bose & Fermi gas behave very differently and we'll consider them in more detail.