Quantum Statistics in the Grand Canonical Ensemble

$$\hat{H}_N = \underbrace{\sum_i h(i)} + \frac{1}{2}\sum_{ij} v(|\mathbf{r}_i - \mathbf{r}_j|)$$

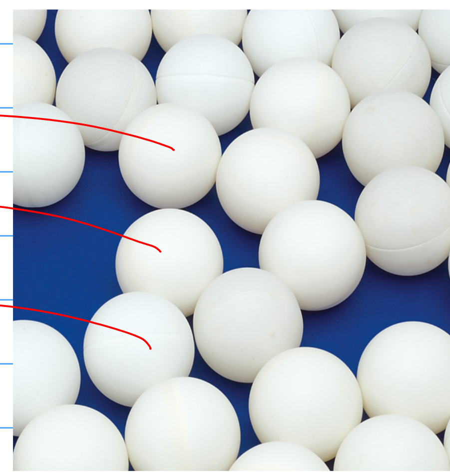
Hilbert space: $\mathcal{H}_N = \text{Span}\{|x_1\rangle \dots |x_N\rangle\}$

Fock space: $\mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3 \oplus \dots$

$$|\chi_j\rangle \qquad |\chi_j\rangle \otimes |\chi_k\rangle$$

$$|\underset{j=1}{n_1} \;\dots\dots\; \underset{j=\infty}{n_\infty} \dots\rangle$$

If $n_j = 0$: leave out.



$|\chi_j\rangle$ (spin) Orbitals

$\langle x_i|$ particles

n_j particles go into drawer j (or $|\chi_j\rangle$).

$$Z_{gr.} = \sum_N e^{\beta\mu N} \sum_{\{n_j\}_N} e^{-\beta\sum_k n_k \epsilon_k}$$

$$= \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \dots \sum_{n_j=0}^{\infty} \dots e^{\beta\mu\sum_k n_k} e^{-\beta\sum_k n_k \epsilon_k}$$

$$= \sum_{n_1=0}^{\infty} e^{\beta(\mu-\epsilon_1)n_1} \sum_{n_2=0}^{\infty} e^{\beta(\mu-\epsilon_2)n_2} \cdots\cdots$$

$$= \prod_j \sum_{n_j=0}^{\infty} e^{\beta(\mu-\epsilon_j)n_j}$$

$$\sum_{n_j} e^{\beta(\mu-\epsilon_j)n_j} = 1 + e^{\beta(\mu-\epsilon_j)}$$ Fermions $(n_j = 0, 1)$

$$= \frac{1}{1 - e^{\beta(\mu-\epsilon_j)}}$$ Bosons

$\mu - \epsilon_j < 0$!

$$\langle n_k \rangle = \frac{\sum_{n_1} e^{\beta(\mu-\epsilon_1)n_1} \cdots \sum_{n_k} e^{\beta(\mu-\epsilon_k)n_k} n_k \cdots\cdots}{\sum_{n_1} e^{\beta(\mu-\epsilon_1)n_1} \cdots \sum_{n_k} e^{\beta(\mu-\epsilon_k)n_k} \cdots\cdots}$$

$$= \frac{\sum_{n_k} e^{\beta(\mu-\epsilon_k)n_k} n_k}{\sum_{n_k} e^{\beta(\mu-\epsilon_k)n_k}} = \frac{\partial}{\partial(\beta\mu)} \log\left(\sum_{n_k} e^{\beta(\mu-\epsilon_k)n_k}\right)$$

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

$$= \frac{e^{\beta(\mu-\epsilon_k)}}{1 - e^{\beta(\mu-\epsilon_k)}} = \frac{1}{e^{\beta(\epsilon_k-\mu)} - 1}$$

For completeness: Maxwell Boltzmann Counting.

$$Z_{gr} = \prod_j \sum_{\{n_j\}} \frac{1}{n_j!} e^{\beta(\mu-\epsilon_j)n_j} = \prod_j e^{e^{\beta(\mu-\epsilon_j)}}$$

$$n_k = -\frac{\partial \ln Z_{gr}}{\partial(\beta\epsilon_k)} = -\frac{\partial \sum_j e^{\beta(\mu-\epsilon_j)}}{\partial(\beta\epsilon_k)} = e^{\beta(\mu-\epsilon_k)}$$