Chapter 5 : Noninteracting Quantum Systems

Quantum many-body Hamiltonian :

$$\hat{H}_0 = \sum_{i=1}^{N} \left\{ \frac{\hat{\vec{p}}_i^{\,2}}{2m} + V(\hat{\vec{x}}_i) \right\} = \sum_{i=1}^{N} \hat{h}(\hat{\vec{x}}_i, \hat{\vec{p}}_i)$$

with $[\hat{x}_i^{\alpha}, \hat{p}_j^{\beta}] = i\hbar\,\delta_{ij}\,\delta^{\alpha\beta}$

Interacting : $\hat{H} = \hat{H}_0 + \sum_{i<j} U(|\hat{\vec{x}}_i - \hat{\vec{x}}_j|)$

"Second Quantization" :

$$\hat{H}_0 = \sum_{\alpha} \varepsilon_{\alpha}\, \hat{n}_{\alpha}$$

where $\hat{h}|\alpha\rangle = \varepsilon_{\alpha}|\alpha\rangle$, i.e. $|\alpha\rangle$ is a 1-particle eigenstate (of $\hat{h}$), thus $\{\varepsilon_{\alpha}\} = \mathrm{spec}(\hat{h})$, and $\hat{n}_{\alpha}$ = # of particles in state $|\alpha\rangle$.

$$\Psi(\vec{x}_1, \ldots, \vec{x}_N) \longrightarrow |\{n_{\alpha}\}\rangle = |\vec{n}\rangle$$

$$\hat{n}_{\alpha}|\vec{n}\rangle = n_{\alpha}|\vec{n}\rangle$$

$\hat{n}_\alpha$ = # operator for state α

n_α = eigenvalue of $\hat{n}_\alpha$

$$\hat{H}_0 |\vec{n}\rangle = \sum_\alpha \varepsilon_\alpha n_\alpha |\vec{n}\rangle$$

Bosons and fermions:

Two types of quantum particle:

- bosons $\Rightarrow$ $n_\alpha \in \{0, 1, 2, \dots\}$
- fermions $\Rightarrow$ $n_\alpha \in \{0, 1\}$

"Pauli exclusion principle"

E.g. $\alpha = (k_x, k_y, k_z) \rightarrow (l_x, l_y, l_z)$

$$k_x = \frac{2\pi l_x}{L_x} \quad \text{etc.}$$

with spin: $(l_x, l_y, l_z, \underbrace{\sigma}_{\pm 1})$

OCE : $Z(T,V,N) = \sum_{\{n_\alpha\}} e^{-\beta \sum_\alpha n_\alpha \varepsilon_\alpha} \delta_{\sum_\alpha n_\alpha, N}$

1D SHO : states $|0\rangle, |1\rangle, \cdots$

Constraint $N = \sum_\alpha n_\alpha$ makes OCE difficult.

So use GCE :

$$\Xi(T,V,\mu) = \sum_N Z(T,V,N)\, e^{\beta\mu N}$$

$$= \sum_{\{n_\alpha\}} e^{\beta \sum_\alpha (\mu - \varepsilon_\alpha) n_\alpha}$$

$$= \sum_{n_1} e^{\beta(\mu-\varepsilon_1)n_1} \sum_{n_2} e^{\beta(\mu-\varepsilon_2)n_2} \cdots$$

Suppose $\alpha = 1,2$. States labeled by (n_1, n_2)

Fermions : $(n_1, n_2) = (0,0), (1,0), (0,1), (1,1)$

$$\rightarrow \sum_{n_1=0}^{1} \times \sum_{n_2=0}^{1}$$

So $\Xi = \prod_\alpha \left(\sum_{n_\alpha} e^{-\beta(\varepsilon_\alpha - \mu) n_\alpha} \right)$

For fermions, $n_\alpha = 0, 1$ so

$$\Xi_{FD} = \prod_\alpha \left[1 + e^{\beta(\mu - \varepsilon_\alpha)} \right]$$

Fermi - Dirac statistics

For bosons,

$$\Xi_{BE} = \prod_\alpha \sum_{n_\alpha = 0}^{\infty} e^{\beta(\mu - \varepsilon_\alpha) n_\alpha}$$

Bose - Einstein statistics

Recall $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$

$$S = (1 + x + x^2 + \dots)$$

$$(1-x) S = 1 \cancel{-x} \cancel{+x} \cancel{-x^2} \cancel{+x^2} \cancel{-x^3} + \dots$$

$$S = \frac{1}{1-x} \quad \text{if } |x| < 1$$

$$\Xi_{BE} = \prod_\alpha \frac{1}{1 - e^{\beta(\mu - \varepsilon_\alpha)}}, \quad \mu < \varepsilon_\alpha \ \forall \alpha$$

Put it all together:

$$\Xi(T,V,N) = e^{-\Omega(T,V,N)/k_BT}$$

$$\left\{\begin{matrix} BE \\ FD \end{matrix}\right\} \quad \Omega(T,V,N) = \pm k_BT \sum_\alpha \log\left(1 \mp e^{-(\varepsilon_\alpha-\mu)/k_BT}\right)$$

Furthermore:

$$\langle \hat{n}_\alpha \rangle = \frac{\partial \Omega}{\partial \varepsilon_\alpha} = \frac{1}{e^{(\varepsilon_\alpha-\mu)/k_BT} \mp 1}$$

$$N = \langle \hat{N} \rangle = \sum_\alpha \langle \hat{n}_\alpha \rangle$$

Maxwell-Boltzmann (classical) limit:

Why isn't

$$Z \stackrel{?}{=} \sum_{\alpha_1} \cdots \sum_{\alpha_N} e^{-\beta(\varepsilon_{\alpha_1}+\cdots+\varepsilon_{\alpha_N})} = \zeta^N$$

where α_j = state of particle j

$(\hat{h}|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle)$; $\zeta = \sum_\alpha e^{-\beta\varepsilon_\alpha}$

True for distinguishable particles.