Identical Particles

N particles with identical properties (mass, spin, ...)

noninteracting particles

$$H = \sum_{i=}^{N} H_n$$

$$H_n = \frac{1}{2m}\vec{P}_n^2 + \underbrace{H_{n,int}}_{\text{spins, vibrations, rotations, etc.}}$$

single-particle quantum states: $|(i)\rangle$

energy eigenstates: $H|(i)\rangle = \varepsilon_i |(i)\rangle$

can be labeled by momentum $\vec{p}$ and discrete quantum numbe

$$(i) = (\vec{p}, m_s, n, l, m_l, \ldots)$$

particle in cubic box of length L with periodic boundary conditions (unphysical, mathematically simple, correct thermodynamic limit)

$\Longrightarrow$ discrete momenta: $\vec{p} = \frac{2\pi\hbar}{L}(n_x, n_y, n_z)$

$n_x, n_y, n_z = 0, \pm 1, \pm 2, \ldots$

N distinguishable particles

basis states are all possible direct products of single-particle basis states

$$|(i_1),(i_2),\ldots,(i_N)\rangle$$

$$\hat{H}|(i_1),\ldots,(i_N)\rangle = \left(\sum_{n=1}^{N} \varepsilon_n\right)|(i_1),\ldots,(i_N)\rangle$$

N identical fermions

quantum state must be

antisymmetric under interchange of any two particles

$\begin{pmatrix}\text{even}\\ \text{odd}\end{pmatrix}$ under any $\begin{pmatrix}\text{even}\\ \text{odd}\end{pmatrix}$ permutation of particle

normalized basis states

$$\frac{1}{\sqrt{N!}}\sum_{P}(-1)^P\, P\,|(i_1),(i_2),\ldots,(i_N)\rangle \qquad (i_1),\ldots,(i_N) \text{ distinct}$$

sum over $N!$ permutations

complication: N single-particle state must be distinct

N identical bosons

quantum state must be

symmetric under interchange of any 2 particles

even under any permutation of particles

normalized basis state

$$\frac{1}{\sqrt{N!}} \sum_P P \left| (i_1), (i_2), \ldots, (i_N) \right\rangle \quad \text{if } (i_1), \ldots, (i_N) \text{ all distinct}$$

sum over $N!$ permutations

$$\frac{1}{2\sqrt{(N-2)!}} \sum_P P \left| (i_1), (i_1), (i_3), \ldots, (i_N) \right\rangle \quad (i_1), (i_3), \ldots, (i_N) \text{ distinct}$$

$\vdots$

$$\frac{1}{N!} \sum_P P \left| (i_1), (i_1), \ldots, (i_N) \right\rangle = \left| (i_1), (i_1), \ldots, (i_1) \right\rangle$$

complication: normalization factor depends on how many of the (i_n) are same

Ideal gas of N identical atoms

$$\hat{H} = \sum_{n=1}^{N} \frac{1}{2m} \vec{P}_n^{\,2}$$

cubic box of length L with periodic boundary condition

single-particle quantum states: $|\vec{n}\rangle = |(n_x, n_y, n_z)\rangle$

$n_x, n_y, n_z = 0, \pm 1, \pm 2, \ldots$

momentum: $\vec{P}_1 |\vec{n}\rangle = \frac{2\pi\hbar}{L}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} |\vec{n}\rangle = \left(\frac{2\pi\hbar}{L}\vec{n}\right)|\vec{n}\rangle$

energy: $H_1 |\vec{n}\rangle = \frac{1}{2m}\vec{P}_1^{\,2} |\vec{n}\rangle = \varepsilon(\vec{n})|\vec{n}\rangle \quad \varepsilon(\vec{n}) = \frac{2\pi^2\hbar^2}{mL^2}(n_x^2 + n_y^2 + n_z^2)$

Canonical ensemble for N identical fermions

at temperature $T = 1/\beta$

partition function: $Z_N = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right]$

direct product basis: $\frac{1}{\sqrt{N!}} \sum_P (-1)^P P |\vec{n}_1, \vec{n}_2, \ldots, \vec{n}_N\rangle \quad \vec{n}_1, \ldots, \vec{n}_N$ distinct

$$Z_N^{\text{fermion}} = \frac{1}{N!} \underbrace{\sum_{\vec{n}_1} \cdots \sum_{\vec{n}_N}}_{\text{distinct}} \left(\frac{1}{\sqrt{N!}} \sum_{P'} (-1)^{P'} \langle \vec{n}_1, \ldots, \vec{n}_N | \overleftarrow{P'} \right)$$

$$\times e^{-\beta\hat{H}} \left(\frac{1}{\sqrt{N!}} \sum_P (-1)^P P |\vec{n}_1, \ldots, \vec{n}_N\rangle \right)$$

$$= \frac{1}{N!}\left(\frac{1}{\sqrt{N!}}\right)^2 \sum_{\vec{n}_1, \ldots, \vec{n}_N}{}' e^{-\beta \sum_{n=1}^{N} \varepsilon(\vec{n}_n)} \underbrace{\sum_{P'} (-1)^{P'} \sum_P (-1)^P \underbrace{\langle \vec{n}_1, \ldots, \vec{n}_N | P' P | \vec{n}_1, \ldots \rangle}_{\delta_{P'P}}}_{\sum_P (-1)^{2P} = N!}$$

$$Z_N^{fermion} = \frac{1}{N!} \sum_{\vec{n}_1, \ldots, \vec{n}_N}{}' \exp\left(-\beta \sum_{n=1}^{N} \varepsilon(\vec{n}_n)\right)$$

sum over distinct vectors $\vec{n}_1, \ldots, \vec{n}_N$

Gibbs factor

classical limit (high temperature)

ignore constraint that $\vec{n}_1, \ldots, \vec{n}_N$ must be distinct

$$Z_N^{fermion} \simeq \frac{1}{N!} \sum_{\vec{n}_1} \cdots \sum_{\vec{n}_N} \exp\left(-\beta \frac{2\pi\hbar^2}{mL^2} (\vec{n}_1^{\,2} + \cdots + \vec{n}_N^{\,2})\right)$$

$$= \frac{1}{N!} \left[\sum_{\vec{n}} \exp\left(-\beta \frac{2\pi\hbar^2}{mL^2} \vec{n}^{\,2}\right)\right]^N$$

approximate sums over n_x, n_y, n_z by integral over p_x, p_y, p_z

$$Z_N^{fermion} \simeq \frac{1}{N!} \left[\left(\frac{L}{2\pi\hbar}\right)^3 \int d^3p_x \exp\left(-\beta \frac{\vec{p}^{\,2}}{2m}\right)\right]^N$$

$$= \frac{1}{N!} \left[\frac{V}{(2\pi\hbar)^3} \left(\sqrt{\frac{2\pi m}{\beta}}\right)^3 \right]^N$$

$$= \frac{1}{N!} \left[\frac{V}{\lambda_{th}^3} \right]^N \qquad \lambda_{th} = \sqrt{\frac{2\pi\hbar^2}{mkT}}$$

$$= Z_N^{classical}$$

Canonical ensemble for N identical bosons at temperature $T = 1/\beta$

$$Z_N^{boson} = \frac{1}{N!} \underbrace{\sum_{\vec{n}_1} \cdots \sum_{\vec{n}_N}}_{distinct} \left(\frac{1}{\sqrt{N!}} \sum_{P'} \langle \vec{n}_1, \ldots, \vec{n}_N | \overleftarrow{P'} \right) e^{-\beta H} \left(\frac{1}{\sqrt{N!}} \sum_{P} P | \vec{n}_1, \ldots, \vec{n}_N \rangle \right)$$

+ terms with 2 same $\vec{n}_n$ and $(N-2)$ distinct

+ " 3 " $N-3$ "

+ ...

+ terms with all $\vec{n}_n$ the same

classical limit (high temperature)

ignore all terms with same $\vec{n}_i$

$$Z_N^{boson} \simeq \frac{1}{N!} \sum_{\vec{n}_1} \cdots \sum_{\vec{n}_N} \left(\frac{1}{\sqrt{N!}} \sum_{P'} \langle \vec{n}_1, \ldots, \vec{n}_N | \overleftarrow{P'} \right) e^{-\beta H} \left(\frac{1}{\sqrt{N!}} \sum_{P} P | \vec{n}_1, \ldots, \vec{n}_N \rangle \right)$$

$$= \frac{1}{N!} \left(\frac{1}{\sqrt{N!}} \right)^2 \sum_{\vec{n}_1} \cdots \sum_{\vec{n}_N} e^{-\beta \sum_{n=1}^{N} \varepsilon(\vec{n}_n)} \underbrace{\sum_{P'} \sum_{P} \langle \vec{n}_1, \ldots, \vec{n}_N | P' P | \vec{n}_1, \ldots, \vec{n}_N \rangle}_{\delta_{P'P}}$$

$$\sum_P 1 = N!$$

$$= \frac{1}{N!} \sum_{\vec{n}_1} \cdots \sum_{\vec{n}_N} e^{-\beta \sum_{n=1}^{N} \varepsilon(\vec{n}_n)}$$

$$= Z_N^{classical}$$

effect of identical particle
can be reproduced in the classical limit
by a temperature-dependent potential $V_\pm(|\vec{r}_1-\vec{r}_2|;T)$
between the particle

$$V_\pm(r;T) = -kT\log\left(1\pm e^{-2\pi r^2/\lambda_{th}^2}\right) \qquad \lambda_{th} = \sqrt{\frac{2\pi\hbar^2}{mkT}}$$

classical partition function

$$Z_2^{\pm} = \frac{1}{2}\,\frac{1}{2\pi\hbar}\int d^3r_1\int d^3p_1 \cdot \frac{1}{2\pi\hbar}\int d^3r_2\int d^3p_2$$

$$\times\, e^{-\beta\left(\frac{1}{2m}p_1^2+\frac{1}{2m}p_2^2\right)}\; \underbrace{e^{-\beta V_\pm(|\vec{r}_1-\vec{r}_2|,T)}}_{1\pm e^{-2\pi(\vec{r}_1-\vec{r}_2)^2/\lambda_{th}^2}}$$

$$= \frac{1}{2}\Bigg(\underbrace{\frac{1}{2\pi\hbar}\int d^3p\, e^{-\beta p^2/2m}}_{\left(\sqrt{\frac{2\pi m}{\beta}}\right)^3}\Bigg)^2 \underbrace{\int d^3r_1\int d^3r_2\left(1\pm e^{-2\pi(\vec{r}_1-\vec{r}_2)^2/\lambda_{th}^2}\right)}_{\int d^3r_1\int d^3r_2 \,\pm\, \int d^3R\int d^3r\, e^{-2\pi r^2/\lambda_{th}^2}}$$

$$= V^2 \pm V\left(\sqrt{\frac{\pi\lambda_{th}^2}{2\pi}}\right)^3$$

$$= \frac{1}{2}\left(\frac{V}{\lambda_{th}^3}\right)^3\left[1\pm\frac{1}{\sqrt{8}}\,\frac{\lambda_{th}^3}{V}\right]$$

effects of identical particles can be reproduced by effective Hamiltonian

$$H_{eff} = \frac{1}{2m}\vec{p}_1^{\,2} + \frac{1}{2m}\vec{p}_2^{\,2} + V_\pm(|\vec{r}_1-\vec{r}_2|;T)$$

first correction from identical particles
comes from pairs of particles

partition function for 2 identical $\begin{pmatrix}\text{bosons}\\ \text{fermions}\end{pmatrix}$

$$\hat{H} = \frac{1}{2m}\vec{P}_1^{\,2} + \frac{1}{2m}\vec{P}_2^{\,2}$$

periodic boundary condition: $\vec{P}_1|\vec{n}_1,\vec{n}_2\rangle = \frac{\pi\hbar}{L}\vec{n}_1|\vec{n}_1,\vec{n}_2\rangle$

$$\vec{P}_2|\vec{n}_1,\vec{n}_2\rangle = \frac{\pi\hbar}{L}\vec{n}_2|\vec{n}_1,\vec{n}_2\rangle$$

$$Z_2^{\pm} = \frac{1}{2}\sum_{\vec{n}_1}\sum_{\vec{n}_2}\frac{1}{\sqrt{2}}\left(\langle\vec{n}_1,\vec{n}_2| \pm \langle\vec{n}_2,\vec{n}_1|\right)e^{-\beta H}\frac{1}{\sqrt{2}}\left(|\vec{n}_1,\vec{n}_2\rangle \pm |\vec{n}_2,\vec{n}_1\rangle\right)$$

$$= \frac{1}{2}\left(\frac{1}{\sqrt{2}}\right)^2\sum_{\vec{n}_1}\sum_{\vec{n}_2}e^{-\beta\left(\varepsilon(\vec{n}_1)+\varepsilon(\vec{n}_2)\right)}\underbrace{\left(\langle\vec{n}_1,\vec{n}_2| \pm \langle\vec{n}_2,\vec{n}_1|\right)\left(|\vec{n}_1,\vec{n}_2\rangle \pm |\vec{n}_2,\vec{n}_1\rangle\right)}_{2 \pm \langle\vec{n}_1\vec{n}_2|\vec{n}_2\vec{n}_1\rangle \pm \langle\vec{n}_2,\vec{n}_1|\vec{n}_1,\vec{n}_2\rangle}$$

$$= \frac{1}{2}\left(\sum_{\vec{n}_1}\sum_{\vec{n}_2}e^{-\beta(\varepsilon(\vec{n}_1)+\varepsilon(\vec{n}_2))} \pm \sum_{\vec{n}_1}e^{-2\beta\varepsilon(\vec{n}_1)}\right)$$

approximate sums over $\vec{n}$ by integral over $\vec{p}$: $\sum_{\vec{n}} \longrightarrow \left(\frac{L}{2\pi\hbar}\right)^3\int d^3p$

$$Z_2^{\pm} = \frac{1}{2}\left[\left(\frac{L}{2\pi\hbar}\right)^6\int d^3p_1\int d^3p_2\, e^{-\beta\left(\frac{1}{2m}\vec{p}_1^{\,2}+\frac{1}{2m}\vec{p}_2^{\,2}\right)}\right.$$

$$\left.\pm\left(\frac{L}{2\pi\hbar}\right)^3\int d^3p\, e^{-2\beta\cdot\frac{1}{2m}\vec{p}^{\,2}}\right]$$

$$= \frac{1}{2}\left[\left(\frac{L}{2\pi\hbar}\right)^6\left(\sqrt{\frac{2\pi m}{\beta}}\right)^6 \pm \left(\frac{L}{2\pi\hbar}\right)^3\left(\sqrt{\frac{\pi m}{\beta}}\right)^3\right]$$

$$= \frac{1}{2}\left[\left(\frac{V}{\lambda_{th}^3}\right)^2 \pm \frac{1}{\sqrt{8}}\left(\frac{V}{\lambda_{th}}\right)\right]$$

In many-body system,
effects of identical particles on pairs of particles
can be reproduced by effective Hamiltonian

$$H_{eff} = \sum_{n=1}^{N} \frac{1}{2m} \vec{P}_n^2 + \sum_{n_1<n_2} V_\pm(|\vec{r}_1 - \vec{r}_2|; T)$$

$$V_\pm(r;T) = -kT \log\left(1 \pm e^{-2\pi r^2/\lambda_{th}^2}\right)$$

$$\lambda_{th} = \sqrt{\frac{2\pi\hbar^2}{mkT}}$$

effective potential: