density op: $\hat{\rho} = \dfrac{e^{-\beta \hat{H}}}{Z}$ $\qquad Z = Tr\,(e^{-\beta \hat{H}})$

$$e^{-\beta \hat{H}} = e^{-\beta \hat{H}}\,\mathbb{1} = e^{-\beta \hat{H}} \sum_k |E_k\rangle\langle E_k| = \sum_k e^{-\beta E_k} |E_k\rangle\langle E_k|$$

density matrix in coord. repr.: N particles, canonical ensemble

$$\langle x | \hat{\rho} | x' \rangle \qquad Tr(\hat{\rho}) = \int dx \langle x | \hat{\rho} | x \rangle = 1$$

$$Z = Tr\left(e^{-\beta \hat{H}}\right) = \int dx \langle x | e^{-\beta \hat{H}} | x \rangle$$

$$\langle x | e^{-\beta \hat{H}} | x' \rangle = \sum_k e^{-\beta E_k} \langle x | E_k \rangle \langle E_k | x' \rangle =$$

$$\boxed{= \sum_k e^{-\beta E_k} \psi_k(x)\, \psi_k^*(x')}$$

$x = \bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N$
$k = \bar{k}_1, \bar{k}_2, \ldots, \bar{k}_N$

N free and <u>indistinguishable</u> particles, in a box, $V = L^3$

single particle wave function $\Rightarrow$ $\boxed{\varphi_{\bar{k}_i}(\bar{x}_i) = \dfrac{1}{\sqrt{V}} e^{i \bar{k}_i \cdot \bar{x}_i}}$ $\qquad \bar{k}_i = \dfrac{2\pi}{L} \bar{n}_i \qquad n_i^{x,y,z} = (0, 1, 2, \ldots$

$\boxed{\text{Fermions}}$

$$\psi_{\bar{k}_1 \bar{k}_2 \ldots \bar{k}_N}(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N) = \frac{1}{\sqrt{N!}} \sum_P \delta_P\, \varphi_{\bar{k}_1}(P\bar{x}_1)\, \varphi_{\bar{k}_2}(P\bar{x}_2) \ldots \varphi_{\bar{k}_N}(P\bar{x}_N)$$

$$E_{k_1, k_2, \ldots k_N} = \frac{\hbar^2}{2m}\left(k_1^2 + k_2^2 + \ldots + k_N^2\right) \qquad \delta_P = (\pm 1)^{[P]}$$

for Fermions

$$\langle x_1, x_2, \ldots x_N | e^{-\beta \hat{H}} | x_1', x_2', \ldots, x_N' \rangle =$$

$$\sum_{k_1, k_2, \ldots k_N}' e^{-\frac{\hbar^2}{2m}(k_1^2+k_2^2+\ldots k_N^2)} \times$$

$$\times \frac{1}{N!}\left(\sum_P \delta_P \varphi_{k_1}(Px_1)\varphi_{k_2}(Px_2)\ldots\varphi_{k_N}(Px_N)\right)\times\left(\sum_{\tilde{P}} \delta_{\tilde{P}} \varphi^*_{k_1}(\tilde{P}x_1')\varphi^*_{k_2}(\tilde{P}x_2')\ldots\varphi^*_{k_N}(\tilde{P}x_N')\right)$$

$$= \sum_{k_1, k_2, \ldots, k_N}' e^{-\frac{\beta\hbar^2}{2m}(k_1^2+k_2^2+\ldots+k_N^2)} \times \frac{1}{N!}$$

$$\times\left(\sum_P \delta_P \varphi_{k_1}(P1)\varphi_{k_2}(P2)\ldots\varphi_{k_N}(PN)\right)\times \sum_{\tilde{P}} \delta_{\tilde{P}} \varphi^*_{\tilde{P}k_1}(1')\varphi^*_{\tilde{P}k_2}(2')\ldots\varphi^*_{\tilde{P}k_N}(N')$$

(extend $\sum'_{k_1 k_2 \ldots k_N}$ to over all k_i permutations: $\sum_{k_1, k_2, \ldots k_N}$ and keep only the first term in the $\sum_{\tilde{P}}$ summation)

$$= \frac{1}{N!}\sum_{k_1, k_2, \ldots, k_N} e^{-\frac{\beta\hbar^2}{2m}(k_1^2+k_2^2+\ldots+k_N^2)} \sum_P \delta_P \varphi_{k_1}(P1)\varphi^*_{k_1}(1')\,\varphi_{k_2}(P2)\varphi^*_{k_2}(2')\ldots\varphi_{k_N}(PN)\varphi^*_{k_N}(N')$$

$$\left[\sum_{k_i} = \left(\frac{L}{2\pi}\right)^3\int d^3k_i = \frac{V}{(2\pi)^3}\int d^3k_i\right] \qquad \left(\Delta n_i^x = \frac{L}{2\pi}\Delta k_i^x\right)$$

$$= \frac{1}{N!}\frac{V^N}{(2\pi)^{3N}}\int d^3k_1 d^3k_2\ldots d^3k_N\, e^{-\frac{\beta\hbar^2}{2m}(k_1^2+k_2^2+\ldots k_N^2)}\sum_P \delta_P \varphi_{k_1}(P1)\varphi^*_{k_1}(1')\ldots\varphi_{k_N}(PN)\varphi^*_{k_N}(N')$$

$$= \frac{1}{N!}\frac{1}{(2\pi)^{3N}} \sum_P \delta_P \int d^3k_1 \dots d^3k_N \, e^{-\frac{\beta\hbar^2}{2m}(k_1^2+\dots+k_N^2)} e^{ik_1(P1-1')} \dots e^{ik_N(PN-N')}$$

$$= \frac{1}{N!}\frac{1}{(2\pi)^{3N}} \sum_P \delta_P \underbrace{\int d^3k_1 \, e^{-\frac{\beta\hbar^2}{2m}k_1^2 + ik_1(P1-1')}}_{\left(\frac{2\pi mkT}{\hbar^2}\right)^{3/2} e^{-\frac{m}{2\beta\hbar^2}(P1-1')^2}} \dots \int d^3k_N \, e^{-\frac{\beta\hbar^2}{2m}k_N^2 + ik_N(PN-N')}$$

$\hbar = \frac{h}{2\pi}$

$$= \frac{1}{N!}\left(\frac{2\pi mkT}{h^2}\right)^{3N/2} \sum_P \delta_P \, f(P1-1') f(P2-2') \dots f(PN-N')$$

$$f(u) \equiv e^{-\frac{m}{2\beta\hbar^2}u^2} \qquad \lambda \equiv \left(\frac{h^2}{2\pi mkT}\right)^{1/2}$$

True for Bosons as well: with $\delta_P = 1$

diagonal elements:

$$\langle x_1, x_2, \dots, x_N | e^{-\beta\hat{H}} | x_1, x_2, \dots, x_N \rangle = \frac{1}{N!}\frac{1}{\lambda^{3N}} \sum_P \delta_P \, f(Px_1 - x_1) \dots f(Px_N - x_N)$$

$$\boxed{f(u) = e^{-\pi u^2/\lambda^2}}$$

$$Z_N = \int d^3x_1 \dots d^3x_N \, \langle x_1, x_2, \dots, x_N | e^{-\beta\hat{H}} | x_1, x_2 \dots x_N \rangle$$

$$\sum_P \delta_P \, f(Px_1 - x_1) f(Px_2 - x_2) \dots f(Px_N - x_N) = \qquad r_{ij} = |\bar{x}_i - \bar{x}_j|$$

$$= 1 \pm \sum_{i<j} f(r_{ij}) f(r_{ji}) + \dots$$

$$Z_N = \frac{1}{N!}\frac{1}{\lambda^{3N}} \int d^3x_1 d^3x_2 \dots d^3x_N \left\{ 1 \pm \sum_{i<j} f^2(r_{ij}) \right\} =$$

$$= \frac{1}{N!}\frac{1}{\lambda^{3N}} \left\{ V^N \pm \frac{N(N-1)}{2} V^{N-1} \int d^3x \, f^2(x) \right\} = \frac{1}{N!}\frac{V^N}{\lambda^{3N}} \left\{ 1 \pm \frac{N(N-1)}{2V} \int_0^\infty 4\pi r^2 dr f^2(r) \right.$$

$f(r_{ij})$ vanishes rapidly for $\left(\frac{V}{N}\right)^{1/3} \gg \lambda$

classical limit $\quad \lambda^3 \left(\frac{N}{V}\right) \ll 1$

$$Z_N \simeq \frac{1}{N!} \frac{1}{\lambda^{3N}} V^N = \frac{1}{N!} \left(\frac{V}{\lambda^3}\right)^N$$

<u>Illustration</u>: 2 particles

$$e^{-\frac{2\pi |\bar{x}_1 - \bar{x}_2|^2}{\lambda^2}}$$

$$Z_2 = \frac{1}{2} \frac{1}{\lambda^6} \int d^3x_1 \, d^3x_2 \left(1 \pm f^2(\bar{x}_1 - \bar{x}_2)\right)$$

$$= \frac{1}{2} \frac{1}{\lambda^6} \left\{ V^2 \pm V \int d^3x \, f^2(\bar{x}) \right\} = \frac{1}{2} \left(\frac{V^2}{\lambda^3}\right) \left\{ 1 \pm \frac{1}{V} \int_0^\infty 4\pi r^2 dr \, f^2(r) \right\}$$

$$= \frac{1}{2} \left(\frac{V}{\lambda^3}\right)^2 \left\{ 1 \pm \frac{1}{2^{3/2}} \left(\frac{\lambda^3}{V}\right) \right\} \approx \frac{1}{2} \left(\frac{V^2}{\lambda^3}\right)$$

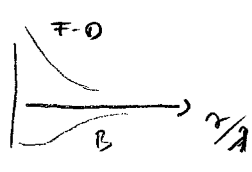
$$\langle x_1, x_2 | \hat{\rho} | x_1, x_2 \rangle = \frac{1}{V^2} \left[1 \pm e^{-\frac{2\pi r_{12}^2}{\lambda^2}} \right]$$

$$\langle x_1, x_2 | e^{-\beta \hat{H}} | x_1, x_2 \rangle = \frac{1}{2\lambda^6} \left\{ 1 \pm e^{-\frac{2\pi r_{12}^2}{\lambda^2}} \right\}$$

$$r_{12} = |\bar{x}_2 - \bar{x}_1|$$

probability density that a pair of particles are separated by a distance r: $\frac{1}{V^2}\left[1 \pm e^{-\frac{2\pi r^2}{\lambda^2}}\right]$

$$v_s = -kT \ln\left(1 \pm e^{-\frac{2\pi r_{12}^2}{\lambda^2}}\right)$$



Summary:

The density operator in the canonical ensemble:

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z} \qquad Z = Tr(e^{-\beta H})$$

$$e^{-\beta \hat{H}} = e^{-\beta \hat{H}} \mathbb{1} = e^{-\beta \hat{H}} \sum_k |k\rangle\langle k|$$

where $\hat{H}|k\rangle = E_k |k\rangle$

$\{|k\rangle\}$ is a complete set of eigenstates of $\hat{H}$

$$e^{-\beta \hat{H}} = e^{-\beta \hat{H}} \sum_k |k\rangle\langle k| = \sum_k e^{-\beta \hat{H}} |k\rangle\langle k| = \sum_k e^{-\beta E_k} |k\rangle\langle k|$$

The matrix elements of the $e^{-\beta \hat{H}}$ operator

$$\langle x| e^{-\beta \hat{H}} |x'\rangle = \langle x| \sum_k e^{-\beta E_k} |k\rangle\langle k| x'\rangle =$$

$$= \sum_k e^{-\beta E_k} \underbrace{\langle x|k\rangle}_{\psi_k(x)} \underbrace{\langle k|x'\rangle}_{\psi_k^*(x')} = \sum_k e^{-\beta E_k} \psi_k(x) \psi_k^*(x')$$

for an N-particle system:

$x = x_1, x_2, \dots, x_N$

k: appropriate set of "good" quantum numbers

for free particles: $k = k_1, k_2, \dots, k_N$

where k_i's are the single-particle quantum numbers.

Density Matrix in Coordinate Representation for $\boxed{\text{Bosons}}$

$$\langle x_1 \dots x_N | \hat{\rho} | x_1' \dots x_N' \rangle = \frac{1}{Z} \langle x_1 \dots x_N | e^{-\beta \hat{H}} | x_1' \dots x_N' \rangle$$

in the canonical ensemble, where $Z = \mathrm{Tr}(e^{-\beta \hat{H}})$

The normalized fully symmetric boson wave function for N particle

$$\psi_{k_1 k_2 \dots k_N}(x_1, x_2, \dots x_N) = \sqrt{\frac{n_1! n_2! \dots}{N!}} \sum_P{}' \underbrace{\varphi_{k_1}(Px_1) \varphi_{k_2}(Px_2)}_{n_1} \dots \underbrace{\varphi_{k_N}(Px_N)}_{n_2} \dots$$

where $n_1, n_2, \dots$ are the number of k_i wave vectors which have the same value, and $\sum'$ runs over the permutations in which particles do not remain in the same state.

Thus, different N-particle wave functions differ in their partition $(n_\alpha, n_\beta, \dots)$

$$\langle x_1 \dots x_N | e^{-\frac{\beta \hbar^2}{2m}(k_1^2 + k_2^2 + \dots + k_N^2)} | x_1' \dots x_N' \rangle =$$

$$= \sum_{\{n_1, n_2, \dots\}}{}' e^{-\frac{\beta \hbar^2}{2m}(k_1^2 + \dots + k_N^2)} \psi_{k_1 \dots k_N}(x_1, \dots, x_N) \psi^*_{k_1, \dots, k_N}(x_1', \dots, x_N') =$$

$$= \sum_{\{n_1, n_2, \dots\}}{}' e^{-\frac{\beta \hbar^2}{2m}(k_1^2 + \dots k_N^2)} \left(\frac{n_1! n_2! \dots}{N!} \right) \sum_P{}' \varphi_{k_1}(Px_1) \dots \varphi_{k_N}(Px_N) \times$$

$$\times \sum_{\tilde{P}}{}' \varphi^*_{k_1}(\tilde{P}x_1') \dots \varphi^*_{k_N}(\tilde{P}x_N') =$$

$$= \langle x | e^{-\beta \hat{H}} | x' \rangle \quad \text{for short}$$

$$(x \equiv x_1, x_2, \dots, x_N)$$

where $\sum'_{\{n_1, n_2 \ldots\}}$ is a sum over the k_i wave vectors with distinct $(n_1, n_2, \ldots,)$ partitioning

since the exponent $(k_1^2 + k_2^2 + \ldots + k_N^2)$ and the fully symmetric wave functions are insensitive to interchanging k_i's within the group of n_α, we can change this sum to one over <u>all</u> k_i's <u>independently</u>, and compensating by a factor $\dfrac{1}{\left(\dfrac{N!}{n_1! n_2! \ldots}\right)}$

$$\langle x | e^{-\beta H} | x' \rangle = \sum_{k_1, k_2 \ldots k_N} e^{-\frac{\beta \hbar^2}{2m}} \left(\frac{n_1! n_2! \ldots}{N!} \right)^2 \sum_P{}' \varphi_{k_1}(Px_1) \ldots \varphi_{k_N}(Px_N) \times \sum_{\tilde{P}}{}' \varphi^*_{k_1}(\tilde{P}x_1') \ldots \varphi^*_{k_N}(\tilde{P}x$$

also, $$(n_1! n_2! \ldots) \sum_P{}' \underbrace{\varphi_{k_1}(Px_1) \varphi_{k_2}(Px_2) \ldots}_{n_1} \underbrace{\varphi_{k_N}(Px_N)}_{n_2 \ldots} =$$

$$= \sum_P \varphi_{k_1}(Px_1) \varphi_{k_2}(Px_2) \ldots \varphi_{k_N}(Px_N)$$

where the sum now runs over <u>all</u> permutations P

$$\langle x | e^{-\beta H} | x' \rangle = \sum_{k_1, k_2, \ldots k_N} e^{-\frac{\beta \hbar^2}{2m}} \frac{1}{(N!)^2} \left(\sum_P \varphi_{k_1}(Px_1) \ldots \varphi_{k_N}(Px_N) \right) \times \left(\sum_{\tilde{P}} \varphi^*_{\tilde{P}k_1}(x_1') \ldots \varphi_{\tilde{P}k_N}(x_N') \right)$$

(permutations over x_i and k_i's yield the same)

$$= \frac{1}{N!} \sum_{k_1, k_2, \ldots k_N} e^{-\frac{\beta \hbar^2}{2m}} \sum_P \varphi_{k_1}(Px_1) \varphi^*_{k_1}(x_1') \ldots \varphi_{k_N}(Px_N) \varphi^*_{k_N}(x_N')$$

<u>Single-particle</u> wave functions in a 3-dim box with linear size L:

$$\psi_{\bar{k}}(\bar{x}) = \frac{1}{\sqrt{V}} e^{i\bar{k}\cdot\bar{x}} \qquad k^{x,y,z} = \frac{2\pi}{L} n^{x,y,z} \qquad n^{x,y,z} = 0,1,2,\ldots$$

$$\sum_{\bar{k}} = \sum \left(\frac{L}{2\pi}\right)^3 (\Delta k)^3 \to \frac{V}{(2\pi)^3} \int d^3k$$

$$\langle x_1 x_2 \ldots x_N | e^{-\beta \hat{H}} | x_1' x_2' \ldots x_N' \rangle = \frac{1}{N!} \frac{V^N}{(2\pi)^{3N}} \int d^3k_1 d^3k_2 \ldots d^3k_N \; e^{-\frac{\beta\hbar^2}{2m}(k_1^2 + k_2^2 + \ldots + k_N^2)} \times$$

$$\times \sum_P \frac{1}{V} e^{i\bar{k}_1(P\bar{x}_1 - \bar{x}_1')} \frac{1}{V} e^{i\bar{k}_2\cdot(P\bar{x}_2 - \bar{x}_2')} \ldots \frac{1}{V} e^{i\bar{k}_N\cdot(P\bar{x}_N - \bar{x}_N')} =$$

$$= \frac{1}{N!} \frac{1}{(2\pi)^{3N}} \sum_P \underbrace{\int d^3k_1 \, e^{-\frac{\beta\hbar^2}{2m}k_1^2 + i\bar{k}_1(P\bar{x}_1 - \bar{x}_1')}}_{\left(\frac{2\pi mkT}{\hbar^2}\right)^{3/2} e^{\frac{-m}{2\beta\hbar^2}(P\bar{x}_1 - \bar{x}_1')^2}} \ldots \int d^3k_N \, e^{-\frac{\beta\hbar^2}{2m}k_N^2 + i\bar{k}_N(P\bar{x}_N - \bar{x}_N')}$$

$$= \frac{1}{N!} \left(\frac{2\pi mkT}{h^2}\right)^{\frac{3N}{2}} \sum_P f(P\bar{x}_1 - \bar{x}_1') f(P\bar{x}_2 - \bar{x}_2') \ldots f(P\bar{x}_N - \bar{x}_N')$$

where $f(u) \equiv e^{-\frac{m}{2\beta\hbar^2}u^2} = e^{-\frac{\pi u^2}{\lambda^2}}$

thermal wavelength: $\lambda \equiv \left(\frac{h^2}{2\pi mkT}\right)^{1/2}$

$$\boxed{\langle x_1 \ldots x_N | e^{-\beta \hat{H}} | x_1' \ldots x_N' \rangle = \frac{1}{N!} \frac{1}{\lambda^{3N}} \sum_P f(P\bar{x}_1 - \bar{x}_1') f(P\bar{x}_2 - \bar{x}_2') \ldots f(P\bar{x}_N - \bar{x}_N')}$$

This is identical to what we obtained for fermions, except for the $\delta_P = (-1)^{[P]}$ in the $\sum_P$ summation

Thus, <u>the general result is</u> :

$$\langle x_1 x_2 \dots x_N | e^{-\beta \hat{H}} | x_1' x_2' \dots x_N' \rangle =$$

$$= \frac{1}{N!} \frac{1}{\lambda^{3N}} \sum_P \delta_P \, f(P\bar{x}_1 - \bar{x}_1') \, f(P\bar{x}_2 - \bar{x}_2') \dots f(P\bar{x}_N - \bar{x}_N')$$

where $\delta_P = 1$ for bosons
and $\delta_P = (-1)^{[P]}$ for fermions ($[P]$ is the order of the permutation)

$$Z_N = Tr(e^{-\beta \hat{H}}) = \int d^3x_1 \, d^3x_2 \dots d^3x_N \, \langle x_1 x_2 \dots x_N | e^{-\beta \hat{H}} | x_1 x_2 \dots x_N \rangle$$

(trace is a sum (integral when continuous variables) over the "diagonal" elements)

Second Quantization, Particle-Number Representation

$$\Psi_{\underbrace{k_1 k_2}_{n_1} \underbrace{\ldots}_{n_2 \ldots} k_N}(\bar{x}_1, \bar{x}_2, \ldots \bar{x}_N) = \langle \bar{x}_1 \bar{x}_2 \ldots \bar{x}_N | n_1\, n_2 \ldots \rangle$$

B: $n_i = 0, 1, 2, \ldots$

F $n_i = 0, 1$

$$a_i |n_1, n_2, \ldots, n_i \ldots \rangle = \sqrt{n_i}\, |n_1, n_2 \ldots n_i - 1 \ldots \rangle$$
$$a_i^+ |n_1 n_1 \ldots n_i \ldots \rangle = \sqrt{n_i + 1}\, |n_1\, n_1 \ldots (n_i + 1) \ldots \rangle$$

B: $[a_i, a_j^+] = \delta_{ij}$ $\qquad [a_i, a_j] = [a_i^+, a_j^+] = \emptyset$

$$|n_1 n_2 \ldots n_i \ldots \rangle = \frac{1}{\sqrt{n_1! n_2! \ldots n_i!}} (a_1^+)^{n_1} (a_2^+)^{n} \ldots \underbrace{|0\rangle}_{|000\ldots0\rangle}$$

F: $\{a_i, a_j^+\} = \delta_{ij}$ $\qquad \{a_i, a_j\} = \{a_i^+, a_j^+\} = \emptyset$

$\{a, b\} \equiv ab + ba$ $\qquad a_i^2 = 0 \qquad (a_i^+)^2 = 0$

$$\hat{n}_i = a_i^+ a_i$$

Bose particles

$$\psi_{\underbrace{k_1 k_2}_{n_1}\underbrace{\dots}_{n_2} k_N}(x_1, x_2, \dots, x_N) = \sqrt{\frac{n_1! n_2! \dots}{N!}} \sum_P{}' \underbrace{\varphi_{k_1}(Px_1)\varphi_{k_2}(Px_2)}_{n_1} \dots \underbrace{\varphi_{k_N}(Px_N)}_{n_2 \dots}$$

$\sum_P{}'$ is sum over permutation in which particles do not remain in the same state

Clearly, the relevant degree of freedom is the set of $\{n_1, n_2, n_3, \dots\}$ occupation numbers the number of particles "n_i" in state "i".

Fermi-Dirac particles

$$\psi_{k_1 k_2 \dots k_N}(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_P \delta_P \, \varphi_{k_1}(Px_1)\varphi_{k_2}(Px_2) \dots \varphi_{k_N}(Px_N) \qquad \delta_P = (-1)^{[P]}$$

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{k_1}(x_1) & \varphi_{k_1}(x_2) & \dots & \varphi_{k_1}(x_N) \\ \varphi_{k_2}(x_1) & \varphi_{k_2}(x_2) & \dots & \varphi_{k_2}(x_N) \\ \vdots & \vdots & & \vdots \\ \varphi_{k_N}(x_1) & \varphi_{k_N}(x_2) & \dots & \varphi_{k_N}(x_N) \end{vmatrix}$$

Particle number representation:

$|n_1 n_2 \dots \rangle$ is the state where n_1 particle is in state 1, n_2 is in state 2, etc

$\sum_i n_i = N$

states should be choosen by "good" quantum numbers, constituting a complete set of orthonormal basis

This view on the N-particle system forms the basis of second quantization.

$$\hat{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=1}^{N} U(x_i) + \frac{1}{2}\sum_{i\neq j} v(\bar{x}_i - \bar{x}_j)$$

general interacting N-particle Hamiltonian

$\boxed{\text{Bose particles}}$:

$$a_i |n_1 n_2 \dots n_i \dots \rangle = \sqrt{n_i}\, |n_1 n_2 \dots (n_i - 1) \dots \rangle$$ annihilation

operators

$$a_i^+ |n_1 n_2 \dots n_i \dots \rangle = \sqrt{n_i + 1}\, |n_1 n_2 \dots (n_i + 1) \dots \rangle$$ creation

$$\Rightarrow \quad a_i^+ a_i |n_1 n_2 \dots n_i \dots \rangle = n_i |n_1 n_2 \dots n_i \dots \rangle$$

$a_i^+ a_i$: number operator $\hat{n}_i$

$$a_i a_i^+ |n_1 n_2 \dots n_i \dots \rangle = (n_i + 1) |n_1 n_2 \dots n_i \dots \rangle$$

(commutator) $[a_i, a_j^+] = \delta_{ij}$, $[a_i, a_j] = 0$, $[a_i^+, a_j^+] = 0$

since the many particle system is symmetric under transposition of particle labels

vacuum state: $|0\rangle$ $\quad n_1 = n_2 = \dots n_i \dots = 0 \quad \forall i$

$$\boxed{|n_1 n_2 \dots n_i \rangle = \frac{1}{\sqrt{n_1! n_2! \dots n_i!}} (a_1^+)^{n_1} (a_2^+)^{n_2} \dots (a_i^+)^{n_i} \dots |0\rangle}$$

$\boxed{\text{Fermions}}$ $n_i = 0, 1$

$|0\rangle = |0\,0 \ldots 0 \ldots\rangle \qquad n_i = 0 \qquad \forall i$

$|n_1 n_2 \ldots n_i \ldots\rangle = (a_1^+)^{n_1} (a_2^+)^{n_2} \ldots (a_i^+)^{n_i} \ldots |0\rangle \qquad n_i = 0, 1$

$|\ldots \underset{i}{1} \ldots \underset{j}{1} \ldots\rangle = \ldots a_i^+ \ldots a_j^+ \ldots |0\rangle$

should be antisymmetric for $i \leftrightarrow j$ $\boxed{a_i^+ a_j^+ = -a_j^+ a_i^+}$ $\boxed{\{a_i^+, a_j^+\} =}$

$\Rightarrow$ consistent with $(a_i^+)^2 = a_i^+ a_i^+ = 0$

$|i\rangle \equiv |0\,0 \ldots 0\,\overset{i}{1}\,0 \ldots\rangle = a_i^+ |0\rangle$

$1 = \langle i|i\rangle = \langle 0| a\, a^+ |0\rangle = \langle 0| \underbrace{a|i\rangle}_{= |0\rangle} \qquad \Rightarrow \quad a_i |i\rangle = |0\rangle$

$\boxed{a_i a_j = -a_j a_i}$ $\boxed{\{a_i, a_j\} = \emptyset}$

from the antisymmetry of the wave function. $a_i^+ a_j = -a_j a_i^+ \quad i \neq j$

and $a_i^+ a_i + a_i a_i^+ = \mathbb{1}$

$\Rightarrow \quad \{a_i, a_j^+\} = \delta_{ij}$

$\hat{n}_i = a_i^+ a_i$ also works again

$a^+|0\rangle = |1\rangle \qquad a|0\rangle = \emptyset \qquad a^2 = \emptyset \qquad (a^+)^2 = \emptyset$

$a^+|1\rangle = \emptyset \qquad a|1\rangle = |0\rangle$

$\left.\begin{array}{ll} a^+ a|0\rangle = \emptyset & a a^+|0\rangle = |0\rangle \\ a^+ a|1\rangle = |1\rangle & a a^+|1\rangle = \emptyset \end{array}\right\} \Rightarrow \{a, a^+\} = 1$

$$\boxed{H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=1}^{N} U(\bar{x}_i) + \frac{1}{2}\sum_{i\neq j} V(\bar{x}_i - \bar{x}_j)}$$

$$= \sum_{i=1}^{N} \mathcal{H}(\bar{x}_i) + \frac{1}{2}\sum_{i\neq j} V(r_{ij}) \qquad r_{ij} = |\bar{x}_i - \bar{x}_j|$$

- $\mathcal{H}(\bar{x}_i) = \frac{\bar{p}_i^2}{2m} + U(\bar{x}_i)$ one-body operator
- $V(\bar{x}_i, \bar{x}_j) = V(r_{ij})$ two-body operator

$\varphi_k(\bar{x}) = \langle \bar{x} | k \rangle$ complete orthonormal set of single-particle states

$$\langle k | \mathcal{H} | l \rangle = \int d^3x \, \varphi_k^*(\bar{x}) \, \mathcal{H}(\bar{x}) \, \varphi_l(\bar{x})$$

$$\langle kl | V | mn \rangle = \int d^3x_1 \int d^3x_2 \, \varphi_k^*(\bar{x}_1) \varphi_l^*(\bar{x}_2) V(\bar{x}_1, \bar{x}_2) \varphi_m(\bar{x}_2) \varphi_n(\bar{x}_1)$$

$|n_1 n_2 \ldots n_i \ldots n_j \ldots \rangle$ properly symmetrized N-particle state $\left(\sum_i n_i = N\right)$

$$a_i |n_1 n_2 \ldots n_i \ldots n_j \ldots \rangle = \sqrt{n_i} \, |n_1 n_2 \ldots (n_i - 1) \ldots n_j \ldots \rangle$$

$$a_i^+ |n_1 n_2 \ldots n_i \ldots n_j \ldots \rangle = \sqrt{n_i + 1} \, |n_1 n_2 \ldots (n_i + 1) \ldots n_j \ldots \rangle$$

$$\Psi_{\underbrace{k_1}_{n_1} \underbrace{k_2}_{n_2} \ldots k_N}(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N) = \langle \bar{x}_1 \bar{x}_2 \ldots \bar{x}_N | n_1 n_2 \ldots \rangle$$

For one-particle operators: $\underbrace{k_1 k_1}_{n_1} \underbrace{\cdots}_{n_2 \cdots} k_N$

$$\langle n_1 n_2 \ldots | \sum_{\substack{i=1 \\ (\text{particles})}}^{N} \mathcal{H}(i) | n_1' n_2' \ldots \rangle = \int d^3x_1 \ldots d^3x_N \, \psi^*_{k_1 k_2 \ldots k_N}(\bar{x}_1, \bar{x}_2, \ldots \bar{x}_N) \sum_{i=1}^{N} \mathcal{H}(\bar{x}_i) \, \psi_{k_1' k_2' \ldots k_N'}(\bar{x}_1, \bar{x}_2, \ldots \bar{x}_N)$$

$$= N \int d^3x_1 d^3x_2 \ldots d^3x_N \, \psi^*_{k_1 k_2 \ldots k_N}(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N) \, \mathcal{H}(\bar{x}_1) \, \psi_{k_1' k_2' \ldots k_N'}(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N)$$

$$\vdots$$

$$\langle n_1 n_2 \ldots | \sum_{k,l} \langle k | \mathcal{H} | l \rangle a_k^+ a_l | n_1' n_2' \ldots \rangle =$$

$$= \sum_{k,l} \langle k | \mathcal{H} | l \rangle \langle n_1 n_2 \ldots n_k \ldots n_l \ldots | a_k^+ a_l | n_1' n_2' \ldots n_k' \quad n_l' \rangle$$

Thus in number representation:

$$\boxed{\sum_{\substack{i=1 \\ (\text{particles})}}^{N} \mathcal{H}(\bar{x}_i) \iff \sum_{k,l} \langle k | \mathcal{H} | l \rangle a_k^+ a_l}$$

For two-particle operators:

$$\boxed{\frac{1}{2} \sum_{\substack{i \neq j \\ (\text{particles})}} V(\bar{x}_i, \bar{x}_j) \iff \frac{1}{2} \sum_{k,l,m,n} \langle k l | V | m n \rangle a_k^+ a_l^+ a_m a_n}$$

$$\hat{H} = \sum_{k,l} \langle k | \mathcal{H} | l \rangle a_k^+ a_l + \frac{1}{2} \sum_{k,l,m,n} \langle k l | V | m n \rangle a_k^+ a_l^+ a_m a_n$$

in particle number representation

Quantized Fields

field operators: $|i\rangle$ single particle states, complete orthonorm
$\langle \bar{x} | i \rangle = \varphi_i(\bar{x})$

$$\boxed{\begin{aligned} \psi(\bar{x}) &= \sum_i \varphi_i(\bar{x})\, a_i \\ \psi^+(\bar{x}) &= \sum_i \varphi_i^*(\bar{x})\, a_i^+ \end{aligned}}$$

$$a_i = \int \varphi_i^*(\bar{x}) \psi(\bar{x})\, d^3x$$

$$a_i^+ = \int \varphi_i(\bar{x}) \psi^+(\bar{x})\, d^3x$$

Boson systems:

$$[\psi(\bar{x}), \psi^+(\bar{x}')] = \delta(\bar{x}-\bar{x}')$$

$$[\psi(\bar{x}), \psi(\bar{x}')] = [\psi^+(\bar{x}), \psi^+(\bar{x}')] = 0$$

Fermions

$$\{\psi(\bar{x}), \psi^+(\bar{x}')\} = \delta(\bar{x}-\bar{x}') \quad , \quad \{\psi(\bar{x}), \psi(\bar{x}')\} = \{\psi^+(\bar{x}), \psi^+(\bar{x}')\} = 0$$

$$\hat{N} = \sum_i a_i^+ a_i = \sum_i \hat{n}_i$$

$$\int \psi^+(\bar{x}) \psi(\bar{x})\, d^3x = \sum_{ij} \underbrace{\int \varphi_i^*(\bar{x}) \varphi_j(\bar{x})\, d^3x}_{\delta_{ij}}\, a_i^+ a_j = \sum_i a_i^+ a_i = \sum_i \hat{n}_i = \hat{N}$$

$\psi^+(\bar{x}) \psi(\bar{x})$ particle density operator $\int \rho(\bar{x})\, d\bar{x} = N$

particle density op. $\rho(\bar{x}) = \sum_{i \,(\text{particles})} \delta(\bar{x}-\bar{x}_i) = \psi^+(\bar{x}) \psi(\bar{x})$

$$\psi(\bar{x}) = \sum_k \varphi_k(\bar{x})\, a_k$$

$$\psi^{+}(\bar{x}) = \sum_k \varphi_k^{*}(\bar{x})\, a_k^{+}$$

$$\hat{H} = \int d^3x\, \psi^{+}(\bar{x})\, \mathcal{H}(\bar{x})\, \psi(\bar{x}) + \frac{1}{2}\iint d^3x_1\, d^3x_2\, \psi^{+}(\bar{x}_1)\psi^{+}(\bar{x}_2)\, V(\bar{x}_1,\bar{x}_2)\,\psi(\bar{x}_2)\psi(\bar{x}_1)$$

$$= \sum_{k,l} \langle k|\mathcal{H}|l\rangle\, a_k^{+} a_l + \frac{1}{2}\sum_{k,l,m,n} \langle kl|V|mn\rangle\, a_k^{+} a_l^{+} a_m a_n$$

$$[\hat{N},\hat{H}] = 0$$

$|k\rangle$ single particle states chosen $\mathcal{H}|k\rangle = \varepsilon_k|k\rangle$

eigenstates of the single-particle Hamiltonian

$$\hat{H} = \sum_k \varepsilon_k\, a_k^{+} a_k + \frac{1}{2}\sum_{k,l,m,n} \langle kl|V|mn\rangle\, a_k^{+} a_l^{+} a_m a_n$$

Ideal (non-interacting) quantum gas

Grand canonical ensemble $\hat{N}, \hat{H}$ in part. num representation

$$\hat{\rho} = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{Z_G} \qquad Z_G = \mathrm{Tr}\left(e^{-\beta(\hat{H}-\mu\hat{N})}\right)$$

$$\hat{H} = \sum_k \varepsilon_k n_k$$

ε_k: spectrum known in principle

$$\hat{N} = \sum_k n_k$$