

2. Identical particles

2.1. Many-Body wave function and particle density

$$P(\vec{R}, t) = |\Psi(\vec{R}, t)|^2 ; \quad P(\vec{R}, t) = \int d\vec{r} \Psi^*(\vec{r}, t) \delta(\vec{R} - \vec{r}) \Psi(\vec{r}, t)$$

$$\hat{n}(\vec{R}) = \delta(\vec{R} - \vec{r})$$

Joint probability density with finding particle 1 at \vec{r}_1 , particle 2 at point $\vec{r}_2, \dots, p.N$ at point \vec{r}_N :

$$P(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = |\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)|^2$$

Particle density operator $\hat{n}(\vec{R}) = \sum_{j=1}^N \delta(\vec{R} - \vec{r}_j)$

Expectation value of $\hat{n}(\vec{R})$:

$$\begin{aligned} n(\vec{R}) &= \int d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_N \Psi^*(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \hat{n}(\vec{R}) \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \\ &= \int d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_N |\Psi(\vec{r}_1, \dots, \vec{r}_N)|^2 \sum_{j=1}^N \delta(\vec{R} - \vec{r}_j) \end{aligned}$$

Consider identical particles : $P(\vec{r}_1, \dots, \vec{r}_N)$ is invariant wrt coordinates permutation:

$$|\Psi(r_1, \dots, r_i, \dots, r_j, \dots, r_N)|^2 = |\Psi(r_1, \dots, r_j, \dots, r_i, \dots, r_N)|^2$$

2.2. Operator of permutations

$$\hat{P}_{ij} \Psi(r_1, \dots, r_i, \dots, r_j, \dots, r_N) = \Psi(r_1, \dots, r_j, \dots, r_i, \dots, r_N)$$

$|\Psi(r_1, \dots, r_N)|^2$ is invariant wrt to \hat{P}_{ij}

For a system of identical particles, operators of observable

(classical limit!) $Z_N = \frac{1}{N!} (Z_1)^N$. Note that the full QM result, $Z = \text{Tr } e^{-\beta \hat{H}}$, differentiates between statistics, as the complete boson functions are different between Bose and Fermi stat. (Huang, Stat. Mech., 2nd edition, Sec. 6.6 and 9.2)

2.3. Exchange energy (example of 2 particles)

$$\hat{H}_0 = \hat{h}(\vec{p}_1, \vec{r}_1) + \hat{h}(\vec{p}_2, \vec{r}_2), \quad \hat{h} = \frac{\vec{p}^2}{2M} + U(\vec{r})$$

$$\hat{h} \Psi_n = \varepsilon_n \Psi_n, \quad n = 0, 1, \dots ; \quad \|\Psi_n\| = 1.$$

$$\Psi_{m,n}^\pm(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} [\Psi_m(\vec{r}_1) \Psi_n(\vec{r}_2) \pm \Psi_m(\vec{r}_2) \Psi_n(\vec{r}_1)]$$

$$\langle \Psi_{m,n}^\pm | \Psi_{m,n}^\pm \rangle = 1 \quad \text{if } \|\Psi_n\| = 1, \text{ and } m \neq n$$

$$m=n: \text{ for fermions } \Psi_{m,m}^- = 0 \quad (\text{Pauli principle})$$

$$\text{for bosons } \Psi_{m,m}^+ = \sqrt{2} \Psi_m(\vec{r}_1) \Psi_m(\vec{r}_2); \text{ to normalize: } \Psi_m = \frac{1}{\sqrt{2!}} \Psi_{m,m}^+$$

Ground state energy for 2 particles:

$$\text{Bosons } \Psi_g = \frac{1}{\sqrt{2!}} \Psi_{0,0}^+ = \Psi_0(\vec{r}_1) \Psi_0(\vec{r}_2); \quad \varepsilon_g = 2\varepsilon_0$$

$$\text{Fermions } \Psi_g = \Psi_{0,1}^-; \quad \varepsilon_g = \varepsilon_0 + \varepsilon_1 \quad \begin{aligned} \Psi_{0,1}^-(\vec{r}_1, \vec{r}_2) \\ = \frac{1}{\sqrt{2}} (\Psi_0(\vec{r}_1) \Psi_1(\vec{r}_2) - \Psi_0(\vec{r}_2) \Psi_1(\vec{r}_1)) \end{aligned}$$

$$\hat{H}_0 \Psi_{m,n} = (\varepsilon_m + \varepsilon_n) \Psi_{m,n} \quad m \neq n; \quad \varepsilon_{m,n}^{(0)} = \varepsilon_m + \varepsilon_n$$

$$\hat{H}_0 \Psi_{m,m} = 2\varepsilon_m \Psi_{m,m}; \quad \varepsilon_{m,m}^{(0)} = 2\varepsilon_m \quad (\text{bosons})$$

Introduce a weak interaction $V(\vec{r}_1 - \vec{r}_2)$ between particles. We want to find corrections to $\varepsilon_{m,n}^{(0)}$ due to interaction.

1st order correction $\delta \varepsilon$ to $\varepsilon_{m,n}^{(0)}$:

$$\begin{aligned} \delta \varepsilon &= \langle \Psi_{m,n}^\pm | \hat{V} | \Psi_{m,n}^\pm \rangle = \frac{1}{2} \int d\vec{r}_1 d\vec{r}_2 | \Psi_m(\vec{r}_1) \Psi_n(\vec{r}_2) \pm \Psi_m(\vec{r}_2) \Psi_n(\vec{r}_1) |^2 V(\vec{r}_1 - \vec{r}_2) \\ &= \frac{1}{2} \int d\vec{r}_1 d\vec{r}_2 (\Psi_m(\vec{r}_1) \Psi_n(\vec{r}_2) \pm \Psi_m(\vec{r}_2) \Psi_n(\vec{r}_1))^* \cdot (\Psi_m(\vec{r}_1) \Psi_n(\vec{r}_2) \pm \Psi_m(\vec{r}_2) \Psi_n(\vec{r}_1)) V(\vec{r}_1 - \vec{r}_2) \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 \left(|\Psi_m(\mathbf{r}_1)|^2 |\Psi_n(\mathbf{r}_2)|^2 + |\Psi_m(\mathbf{r}_2)|^2 |\Psi_n(\mathbf{r}_1)|^2 \right) \cdot V(\mathbf{r}_1 - \mathbf{r}_2) \\
&\quad + \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 \left\{ (\pm i) \Psi_m^*(\mathbf{r}_1) \Psi_n(\mathbf{r}_1) \Psi_n^*(\mathbf{r}_2) \Psi_m(\mathbf{r}_2) + (\mp i) \Psi_m(\mathbf{r}_1) \Psi_n^*(\mathbf{r}_1) \Psi_n(\mathbf{r}_2) \Psi_m^*(\mathbf{r}_2) \right\} \\
&\quad \cdot V(\mathbf{r}_1 - \mathbf{r}_2) \quad \text{density-density interaction} \\
&= \underbrace{\int d\mathbf{r}_1 d\mathbf{r}_2 \left[|\Psi_m(\mathbf{r}_1)|^2 |\Psi_n(\mathbf{r}_2)|^2 - V(\mathbf{r}_1 - \mathbf{r}_2) \right]}_{\pm \int d\mathbf{r}_1 d\mathbf{r}_2 \operatorname{Re} \left\{ (\Psi_m^*(\mathbf{r}_1) \Psi_n(\mathbf{r}_1)) (\Psi_n^*(\mathbf{r}_2) \Psi_m(\mathbf{r}_2)) \right\} \cdot V(\mathbf{r}_1 - \mathbf{r}_2)} \quad \text{(omit vector signs)} \\
&\quad \underbrace{\text{exchange energy}}
\end{aligned}$$

Introduce diagonal $\langle m | \hat{n}(\mathbf{R}) | m \rangle$ and off-diagonal $\langle m | \hat{n}(\tilde{\mathbf{R}}) | n \rangle$ matrix elements of operator $\hat{n}(\tilde{\mathbf{R}})$ for one particle, $\hat{n}(\tilde{\mathbf{R}}) = \delta(\tilde{\mathbf{R}} - \hat{\mathbf{r}})$:

$$n_{mm}(\tilde{\mathbf{R}}) = \langle m | \hat{n}(\tilde{\mathbf{R}}) | m \rangle = |\Psi_m(\tilde{\mathbf{R}})|^2 ; \quad n_{mn}(\tilde{\mathbf{R}}) = \langle m | \hat{n}(\tilde{\mathbf{R}}) | n \rangle = \Psi_m^*(\tilde{\mathbf{R}}) \Psi_n(\tilde{\mathbf{R}})$$

Correction $\delta \varepsilon$ to the state $\varepsilon_{m,n}^{(0)}$:

$$\varepsilon_{m,n} = \varepsilon_{m,n}^{(0)} + \delta \varepsilon,$$

$$\begin{aligned}
\delta \varepsilon &= \langle \Psi_{m,n} | \hat{V} | \Psi_{m,n} \rangle = \underbrace{\int d\mathbf{r}_1 d\mathbf{r}_2 n_{mm}(\mathbf{r}_1) V(\mathbf{r}_1 - \mathbf{r}_2) n_{nn}(\mathbf{r}_2)}_{\text{direct interaction}} \\
&\quad \pm \underbrace{\operatorname{Re} \int d\mathbf{r}_1 d\mathbf{r}_2 n_{mn}(\mathbf{r}_1) V(\mathbf{r}_1 - \mathbf{r}_2) n_{nm}(\mathbf{r}_2)}_{\text{exchange interaction}}
\end{aligned}$$

01.26.23

2.4. N -particle generalizations

a. Fermions

$$\hat{P}_{nm} \Psi(r_1, r_2, \dots, r_n, \dots, r_m, \dots, r_N) = \Psi(r_1, r_2, \dots, r_m, \dots, r_n, \dots, r_N)$$

Fermion wave function satisfies:

$$\hat{P}_{nm} \Psi(r_1, r_2, \dots, r_n, \dots, r_m, \dots, r_N) = (-1)^{\sum_{i=n+1}^m r_i} \Psi(r_1, r_2, \dots, r_n, \dots, r_m, \dots, r_N)$$

To construct a convenient basis for N fermions, consider a orthonormal set of single-particle states $\Psi_j(r_i)$ and

form an antisymmetric combination:

$$\Psi = \frac{1}{\sqrt{N!}} \hat{A} \Psi_{j_1}(r_1) \Psi_{j_2}(r_2) \dots \Psi_{j_N}(r_N)$$

with \hat{A} being the antisymmetrization operator acting on $\{r_i\}$

Introduce operator of permutation:

$$P\{1, 2, 3, \dots, N\} = \{P_1, P_2, P_3, \dots, P_N\} \quad P_k = P(k) \text{ is an image of integer } k$$

Even permutation P : involves an even number of pairwise permutations to achieve $\{P_1, P_2, P_3, \dots, P_N\}$; $(-1)^P = 1$

Odd permutation P : involves an odd number of pairwise permutations to achieve $\{P_1, P_2, P_3, \dots, P_N\}$; $(-1)^P = -1$

Example: $\{1, 2, 3\}$

$$\begin{array}{c} \cancel{\downarrow} \\ \{3, 2, 1\} \text{ odd} \\ \cancel{\downarrow} \\ \{2, 3, 1\} \text{ even} \end{array}$$

$$\Psi = \frac{1}{\sqrt{N!}} \hat{A} \Psi_{j_1}(r_1) \Psi_{j_2}(r_2) \dots \Psi_{j_N}(r_N)$$

$$= \frac{1}{\sqrt{N!}} \sum_{\{P\}} (-1)^P \Psi_{j_1}(r_{P_1}) \Psi_{j_2}(r_{P_2}) \dots \Psi_{j_N}(r_{P_N}) = \frac{1}{\sqrt{N!}} \det M$$

Matrix elements of M : $M_{ij} = \Psi_i(r_j)$

$$\Psi = \frac{1}{\sqrt{N!}} \left| \begin{array}{cccc} \Psi_{j_1}(r_1) & \dots & - & \Psi_{j_1}(r_N) \\ | & & | & | \\ \vdots & & \vdots & \vdots \\ \Psi_{j_N}(r_1) & - & - & \Psi_{j_N}(r_N) \end{array} \right| \quad \text{Slater determinant}$$

We may define Ψ by allowing P to act on $\{j_\ell\}$ instead of $\{r_i\}$:

$$\begin{aligned}\Psi &= \frac{1}{\sqrt{N!}} \hat{A} \Psi_{j_1}(r_1) \Psi_{j_2}(r_2) \cdot \dots \cdot \Psi_{j_N}(r_N) \\ &= \frac{1}{\sqrt{N!}} \sum_{\{P\}} (-1)^P \Psi_{j_{P_1}}(r_1) \cdot \dots \cdot \Psi_{j_{P_N}}(r_N) = \frac{1}{\sqrt{N!}} \det M^T\end{aligned}$$

Matrix elements of M^T : $M_{ij}^T = \Psi_j(r_i)$

$$\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \Psi_{j_1}(r_1) & \dots & \Psi_{j_N}(r_1) \\ \vdots & & \vdots \\ \Psi_{j_1}(r_N) & \dots & \Psi_{j_N}(r_N) \end{vmatrix}$$

The introduced many-body function is normalized:

$$\begin{aligned}\langle \Psi | \Psi \rangle &= \frac{1}{N!} \sum_{\{P\}} \sum_{\{P'\}} (-1)^{P+P'} \prod_{k=1}^N \langle \Psi_{j_{P_k}} | \Psi_{j_{P'_k}} \rangle = \frac{1}{N!} \sum_{\{P\}} \sum_{\{P'\}} (-1)^{P+P'} \delta_{PP'} \\ &= \frac{1}{N!} \sum_{\{P\}} \sum_{\{P'\}} \delta_{PP'} = \frac{1}{N!} \sum_{\{P\}} 1 = 1\end{aligned}$$

Consider a free-fermion system (no interactions)

$$\mathcal{H} = \sum_j h(\hat{p}_j, \hat{r}_j) \quad (\text{symmetric in } (i,j) \text{ for } h(i,j))$$

Pick $\Psi_j(r_j)$ in Ψ as eigenfunctions of $h(\hat{p}_j, \hat{r}_j)$

Suppose Ψ is constructed out of states j_1, j_2, \dots, j_N . The eigenvalues of energy for Ψ is $E = \sum_{k=1}^N \varepsilon_{j_k}$

Introduce occupation numbers of single-particle states n_k (fermions: $n_k = 1$ or 0 depending on whether j_k is present or absent in $\sum \dots$, respectively). We re-write:

$$E = \sum_{k=1}^{\infty} n_k \varepsilon_k, \quad \sum_{k=1}^{\infty} n_k = N.$$

b. Bosons

$$\Psi \propto \sum_{\{P'\}} \psi_{p_1}(r_1) \cdot \dots \cdot \psi_{p_N}(r_N)$$

we should symmetrise wrt different one-particle states.

Introduce here too, the occupation number n_i of state i
(it is the number of coinciding indices in the above Ψ)

The properly normalised function:

$$\Psi = \sqrt{\frac{n_1! n_2! \dots}{N!}} \sum_{\{P'\}} \psi_{p_1}(r_1) \cdot \dots \cdot \psi_{p_N}(r_N)$$

$\{P'\}$: all permutations of different indices. The number of indices p_1, \dots, p_N is $\leq N$.

$$\text{Free-boson system} : E = \sum_{i=1}^{\infty} n_i \epsilon_i ; \quad N = \sum_{i=1}^{\infty} n_i$$

(n_i may take values $0, 1, \dots$)

More: LL v.3, §61 (you may like also §62, c3) + Negele-Orland, Sec. 1.2 and 1.3

3. Second quantization

3.1. Boson statistics (LL v.3, §64)

Let $\psi_1(r), \psi_2(r), \dots$ be a complete orthonormal set of single-particle states (e.g. eigenfunctions of a single-particle Hamiltonian $h(p, r)$).

Introduce occupation numbers n_1, n_2, \dots for states $1, 2, \dots$

We want to construct a formalism operating with $\{n_i\}$ instead of $\{r, \sigma\}_i$:

Use Dirac notations.

$$|n_1, n_2, \dots\rangle = \sqrt{\frac{N! n_k!}{N!}} \sum_{\{P'\}} \psi_{p_1}(r_1) \cdot \dots \cdot \psi_{p_N}(r_N)$$

(representation by occup. #s : Fock space)

Our goal is to evaluate matrix elements of operators of observables in the basis $|n_1, n_2, \dots\rangle$

We start with single-coordinate (single-body) observables:

$$\hat{F}^{(1)} = \sum_a \hat{f}_a^{(1)} = \sum_a f^{(1)}(\hat{r}_a, \hat{p}_a) \quad (\text{a: particle number } a)$$

Example: density operator $\hat{n}(R) = \sum_a \hat{n}^a(R) = \sum_a \delta(R - \hat{r}_a)$

$$\int dr_1 dr_2 \dots dr_a \dots dr_N \psi_i^*(r_1) \psi_1(r_2) \dots \psi_i(r_a) \dots \hat{f}(\hat{p}_a, r_a) \psi_2(r_1) \psi_2(r_2) \dots \psi_k(r_k) \dots$$

$$\hat{n}^a(R) = \delta(R - \hat{r}_a)$$

We are interested in calculating matrix element

$\langle n_1, \dots | F^{(1)} | n'_1, \dots \rangle$ to the matrix elements of $\langle i | f^{(a)} | k \rangle$

$$\langle i | f^{(a)} | k \rangle = \int dr_a \psi_i^*(r_a) f^{(a)}(\hat{r}_a, \hat{p}_a) \psi_k(r_a)$$

$$(\text{example: } n^{(a)}(R) = \delta(R - r_a) \Rightarrow \langle i | n^{(a)}(R) | k \rangle = \int dr_a \psi_i^*(r_a) \delta(R - r_a) \psi_k(r_a))$$

$$\langle i | n^{(a)}(R) | k \rangle = \psi_i^*(R) \psi_k(R)$$

Only one single-particle wave function, each from

$\langle \dots |$ and $| \dots \rangle$ is involved non-trivially in the integration