

Two indistinguishable particles

Wave functions

$$\psi(r_1, r_2) \quad \text{with} \quad \psi(r_2, r_1) = \begin{matrix} \leftarrow \text{bosons} \\ \pm \\ \psi(r_1, r_2) \\ \leftarrow \text{fermions} \end{matrix}$$

basis

for single particle

$$\psi_i(r) \\ |i\rangle$$

for two particles

$$\psi_{ij}(r_1, r_2) = C(\psi_i(r_1)\psi_j(r_2) \pm \psi_j(r_1)\psi_i(r_2))$$

$$|i, j\rangle = C(|i\rangle|j\rangle \pm |j\rangle|i\rangle)$$

$$C = \frac{1}{\sqrt{2}} \quad \text{if } i \neq j$$

4.2 N particles

wave functions $\psi(r_1, r_2, \dots, r_N)$

for bosons: remains the same if two args. are interch.

for fermions: flips sign " " " " "

basis

$$\underbrace{\psi_{i_1 i_2 \dots i_N}}_{\text{occupied single-particle states}}(r_1, r_2, \dots, r_N) = C \left(\psi_{i_1}(r_1) \psi_{i_2}(r_2) \dots \psi_{i_N}(r_N) + \text{terms where indices/args. are interchanged} \right)$$

↑
for fermions each exchange of two indices/arguments leads to a minus sign

normalisation

for fermions:

$$C = \frac{1}{\sqrt{N!}}$$

for bosons

$$C = \frac{1}{\sqrt{N! \prod_i n_i!}}$$

where n_i = number of particles in single-particle state i

4.3 Fock space

can have states that are linear combinations of states with different number of particles

\mathcal{F}_N = Hilbert space of states with N particles

Overall Hilbert space contains lin. comb. of states from different \mathcal{F}_N

$\bigoplus_{N=0}^{\infty} \mathcal{F}_N$ = set of lin. comb. of elements of all \mathcal{F}_N
= Fock space

Contains vacuum state = state with no particles

4.4 Creation + annihilation operators (for bosons)

occupation number representation

$$\underbrace{|1, \dots, 1, 2, \dots, 2, \dots\rangle}_{n_1 \quad n_2} = |n_1, n_2, \dots\rangle$$

corresponding bra: $\langle n_1, n_2, \dots |$

Creation operator: $a_i^\dagger | \dots n_i \dots \rangle = \sqrt{n_i + 1} | \dots n_i + 1 \dots \rangle$

annihilation operator: $a_i | \dots n_i \dots \rangle = \sqrt{n_i} | \dots n_i - 1 \dots \rangle$

Square root factors

- guarantee that $a_i | \dots 0 \dots \rangle = 0$
- consistency with raising/lowering operators for harm. oscillator
- a_i, a_i^\dagger mutually adjoint

Commutators

$$[A, B] = AB - BA$$

Thm: $[a_i, a_j] = 0$, $[a_i^+, a_j^+] = 0$, $[a_i, a_j^+] = \delta_{ij}$

Proof:

• operators with different indices change different occupation numbers and thus commute

• $[a_i, a_i] = 0$, $[a_i^+, a_i^+] = 0$

• $[a_i, a_i^+] | \dots n_i \dots \rangle$

$$= a_i a_i^+ | \dots n_i \dots \rangle - a_i^+ a_i | \dots n_i \dots \rangle$$

$$= a_i \sqrt{n_i + 1} | \dots n_i + 1 \dots \rangle - a_i^+ \sqrt{n_i} | \dots n_i - 1 \dots \rangle$$

$$= (n_i + 1) | \dots n_i \dots \rangle - n_i | \dots n_i \dots \rangle$$

$$= 1 | \dots n_i \dots \rangle$$

Occupation number operator

$$a_i^\dagger a_i | \dots n_i \dots \rangle = n_i | \dots n_i \dots \rangle$$

4.5 Hamiltonian in 2nd quantisation

Example: system with discrete sites

• • • •
1 2 3 4

Single particle Hamiltonian

wave function $\begin{pmatrix} \psi(1) \\ \psi(2) \\ \vdots \end{pmatrix}$

normalisation

$$\sum_i |\psi(i)|^2 = 1$$

Continuous case:

$$(\hat{H}\psi)(x) = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right) \psi(x)$$

here: $\psi'(x) \rightarrow \psi(x+1) - \psi(x)$

$$\psi''(x) \rightarrow \psi'(x) - \psi'(x-1)$$

$$= (\psi(x+1) - \psi(x)) - (\psi(x) - \psi(x-1))$$

$$= \psi(x+1) - 2\psi(x) + \psi(x-1)$$

Hamiltonian:

$$(\hat{H}\psi)(x) = -\frac{\hbar^2}{2m} (\psi(x+1) - 2\psi(x) + \psi(x-1)) + U(x)\psi(x)$$

in matrix form:

$$\hat{H} = -\frac{\hbar^2}{2m} \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & \ddots & \ddots \\ & & \ddots & \ddots \end{pmatrix} + \begin{pmatrix} U(1) & & & \\ & U(2) & & \\ & & \ddots & \\ & & & \ddots \end{pmatrix}$$

Multiple particle Hamiltonian

Wave functions $\psi(x_1, x_2, \dots)$

continuous case:

$$\text{e.g. } \hat{H}_{\text{mult}} = \frac{\hat{p}_1^2}{2m} + U(r_1) + \frac{\hat{p}_2^2}{2m} + U(r_2) + U^{\text{int}}(r_1, r_2)$$

discrete version:

$$\hat{H}_{\text{mult}} = \sum_p \hat{H}_p + \frac{1}{2} \sum_{\substack{p=1..N \\ p'=1..N \\ p \neq p'}} U^{\text{int}}(x_p, x_{p'})$$

↑
acts
w.r.t. x_p

now with creation + annihilation operators

basis: consider states localised at sites

$$\psi_i(x) = \delta_{xi} \quad \left(\begin{array}{c} 1 \\ 0 \\ 0 \\ \vdots \end{array} \right), \left(\begin{array}{c} 0 \\ 1 \\ 0 \\ \vdots \end{array} \right), \dots$$

• potential

$$\sum_i U(i) \underbrace{a_i^\dagger a_i}_{\text{occupation number}}$$

↑
diag. el.

• full single particle Hamiltonian

$$\sum_{ij} H(i, j) a_i^\dagger a_j$$

(no proof)

• interaction potential

$$\frac{1}{2} \sum_{ij} U^{\text{int}}(i, j) \underbrace{a_i^\dagger a_i}_{\text{particles at } i} \left(\underbrace{a_j^\dagger a_j}_{\text{particles at } j} - \underbrace{\delta_{ij}}_{\text{no self interaction}} \right)$$

Thm: $a_i^\dagger a_i (a_j^\dagger a_j - \delta_{ij}) = a_i^\dagger a_j^\dagger a_j a_i$

Proof:

$$\begin{aligned} & a_i^\dagger a_j^\dagger a_j a_i \\ &= a_i^\dagger a_j^\dagger a_i a_j \\ &= a_i^\dagger [a_i a_j^\dagger - \underbrace{(a_i a_j^\dagger - a_j^\dagger a_i)}_{= [a_i, a_j^\dagger] = \delta_{ij}}] a_j \end{aligned}$$

$$= a_i^\dagger a_i (a_j^\dagger a_j - \delta_{ij})$$

□

Total:

$$\hat{H}_{\text{mult}} = \sum_{ij} H(i,j) a_i^\dagger a_j + \frac{1}{2} \sum_{ij} U^{\text{int}}(i,j) a_i^\dagger a_j^\dagger a_j a_i$$

Continuous case

$$i \rightarrow \underline{r}, \quad j \rightarrow \underline{r}'$$

$$a_i^\dagger \rightarrow a^\dagger(\underline{r}), \quad a_j \rightarrow a(\underline{r}), \quad [a(\underline{r}), a^\dagger(\underline{r}')] = \delta(\underline{r} - \underline{r}')$$

Hamiltonian

$$\hat{H} = \int d^n r \, a^\dagger(\underline{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + U(\underline{r}) \right) a(\underline{r}) \\ + \frac{1}{2} \int d^n r \int d^n r' \, U^{\text{int}}(\underline{r}, \underline{r}') a^\dagger(\underline{r}) a^\dagger(\underline{r}') a(\underline{r}') a(\underline{r})$$

Single particle term looks similar to exp. value

$$\int d^n r \, \psi^*(\underline{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + U(\underline{r}) \right) \psi(\underline{r})$$

as if we replaced wavef. by operator (second quantisation)