

Second Quantization (AS)

(Lec. 6) ①

"Occup. # representation"

N particles

$$|Y\rangle = \sum_{m_1, m_2, \dots} C_{m_1, \dots, m_N} |m_1, m_2, \dots, m_N\rangle$$

no need to impose $\sum_i m_i = N$, and admit $|0\rangle$

\Rightarrow Fock space

\rightarrow Spaces w/ $\sum_i m_i = N$

$$\mathcal{F} \equiv \bigoplus_{N=0}^{\infty} \mathcal{F}^N$$

Creation / Annihilation ops. (Bosons)

$$a_i^\dagger |m_1, \dots, m_i, \dots\rangle = (m_i + 1)^{1/2} |m_1, \dots, m_i + 1, \dots\rangle$$

We see that

$$|m_1, m_2, \dots\rangle = \prod_i \frac{1}{(m_i!)^{1/2}} (a_i^\dagger)^{m_i} |0\rangle$$

with also

$$a_i |m_1, m_2, \dots, m_i, \dots\rangle = m_i^{1/2} |m_1, \dots, m_i - 1, \dots\rangle$$

with $[\alpha_i, \alpha_j^\dagger] = \delta_{ij}$; $[\alpha_i, \alpha_j] = 0$
 $[\alpha_i^\dagger, \alpha_j^\dagger] = 0$

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Many-body Quantum Mechanics

characterize state by

$\{|\lambda\rangle\} \rightarrow$ single-particle states

Basis

$$\{|\lambda\rangle\} \rightarrow \{|\tilde{\lambda}\rangle\}$$

$$\Rightarrow \sum_{\lambda} |\lambda\rangle \langle \lambda | \tilde{\lambda} \rangle = |\tilde{\lambda}\rangle$$

But $|\lambda\rangle = \alpha_{\lambda}^{\dagger} |0\rangle$, $|\tilde{\lambda}\rangle = \alpha_{\tilde{\lambda}}^{\dagger} |0\rangle$

$$\Rightarrow \alpha_{\tilde{\lambda}}^{\dagger} |0\rangle = \sum_{\lambda} \langle \lambda | \tilde{\lambda} \rangle \alpha_{\lambda}^{\dagger} |0\rangle$$

$$\text{or } \boxed{\alpha_{\tilde{\lambda}}^{\dagger} = \sum_{\lambda} \langle \lambda | \tilde{\lambda} \rangle \alpha_{\lambda}^{\dagger}}$$

Similarly, $\left\{ \alpha_{\tilde{\lambda}} = \sum_{\lambda} \langle \tilde{\lambda} | \lambda \rangle \alpha_{\lambda} \right\}$

One-body Operators

We can write them as

$$\hat{O}_1 = \sum_{m=1}^N \hat{O}_m$$

\hat{O}_m : single-particle op acting on particle m

Eg: kinetic energy

$$\hat{T} = \sum_m \frac{\hat{p}_m^2}{2m}$$

\hat{p}_m : mom. of acting on particle m

Potential

$$\hat{V} = \sum_m V(\hat{x}_m)$$

Define Occupancy Number Operator

$$\hat{n}_a = a_a^\dagger a_a$$

We can see that

$$\hat{n}_a (a_a^\dagger)^m |0\rangle = m (a_a^\dagger)^m |0\rangle$$

Then

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$$\hat{m}_{r,j} |m_{r_1}, m_{r_2}, \dots\rangle = m_{r,j} |m_{r_1}, m_{r_2}, \dots\rangle$$

$\hat{m}_{r,j}$ counts m_j of particles in state $|r\rangle$.

1-body operator

Assume is diagonal in $\{|r\rangle\}$ basis

$$\Rightarrow \hat{O}_1 = \hat{O}$$

$$\langle m'_{r_1}, m'_{r_2}, \dots | \hat{O}_1 | m_{r_1}, m_{r_2}, \dots \rangle$$

$$= \langle m'_{r_1}, m'_{r_2}, \dots | \sum_i \theta_{r_i} |r_i\rangle \langle r_i| | m_{r_1}, m_{r_2}, \dots \rangle$$
$$= \sum_i \theta_{r_i} \langle m'_{r_1}, m'_{r_2}, \dots | r_i \rangle \langle r_i | m_{r_1}, m_{r_2}, \dots \rangle$$

$$= \langle m'_{r_1}, m'_{r_2}, \dots | \sum_i \theta_{r_i} \hat{m}_{r_i} | m_{r_1}, m_{r_2}, \dots \rangle$$

$$\Rightarrow \hat{O}_1 = \sum_{r=0}^{\infty} \theta_r \hat{a}_r^\dagger \hat{a}_r = \sum_{r=0}^{\infty} \langle r | \hat{O} | r \rangle \hat{a}_r^\dagger \hat{a}_r$$

In a non-diagonal basis

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$$\hat{\theta}_i = \sum_{ij} \langle \alpha_i | \hat{\theta} | \alpha_j \rangle Q_{\alpha_i}^\dagger Q_{\alpha_j}$$

Ex: Free particle

kinetic Energy

$$\hat{T} = \int d^d r Q^\dagger(\vec{r}) \frac{\hat{p}^2}{2m} Q(\vec{r})$$

with $\hat{p} = -i\hbar \nabla$

use to prove:

$$Q(\vec{r}) = \int d^d k \frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}} a_k$$

(or some other normalization of $\frac{1}{\sqrt{V}}$, etc)

\Rightarrow 1-body Hamiltonian is

$$\hat{H} = \int d^d r Q^\dagger(\vec{r}) \left[\frac{\hat{p}^2}{2m} + V(\vec{r}) \right] Q(\vec{r})$$

$V(\vec{r})$: one-particle potential

Density operator :

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Local density op

$$\hat{\rho}(\vec{r}) = a^\dagger(\vec{r}) a(\vec{r})$$

Total occupancy number of

$$\hat{N} = \int d^3r \hat{\rho}(\vec{r}) \quad \left(\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \text{ if discrete spectrum} \right)$$

Two-body Operators

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Describe interaction v

E.g. symmetric 2-body potentials

$$V(\vec{p}_m, \vec{r}_m) = V(\vec{r}_m, \vec{p}_m)$$

Find \hat{V} on 2nd quantized language such that

$$\hat{V} |\vec{p}_1, \vec{p}_2, \dots, \vec{p}_N\rangle = \frac{1}{2} \sum_{m \neq m'} V(\vec{p}_m, \vec{p}_{m'}) |\vec{p}_1, \vec{p}_2, \dots, \vec{p}_N\rangle$$

The answer is

$$\hat{V} = \frac{1}{2} \int d^d r \int d^d r' a^\dagger(\vec{r}) a^\dagger(\vec{r}') V(\vec{r}, \vec{r}') a(\vec{r}') a(\vec{r})$$

To check

$$a^\dagger(\vec{r}) a^\dagger(\vec{r}') a(\vec{r}) a(\vec{r}') |\vec{p}_1, \vec{p}_2, \dots, \vec{p}_N\rangle =$$

$$a^\dagger(\vec{r}) a^\dagger(\vec{r}') \underbrace{a(\vec{r}) a(\vec{r}')}_{\hat{\rho}(\vec{r})} a^\dagger(\vec{p}_1) \dots a^\dagger(\vec{p}_N) |0\rangle$$

$$= \sum_{j=1}^N \delta(\vec{r} - \vec{r}_j) a^\dagger(\vec{r}_j) \hat{\rho}(\vec{r}') a^\dagger(\vec{p}_1) \dots a^\dagger(\vec{p}_{j-1}) a^\dagger(\vec{p}_{j+1}) \dots a^\dagger(\vec{p}_N) |0\rangle$$

$$= \sum_{j=1}^N \delta(\vec{r} - \vec{r}_j) a_{\vec{r}_j}^\dagger \sum_{k \neq j}^N \delta(\vec{r}' - \vec{r}_k) a_{\vec{r}_k}^\dagger \quad (7)$$

$$\times a_{\vec{r}_1}^\dagger \dots a_{\vec{r}_{j-1}}^\dagger a_{\vec{r}_{j+1}}^\dagger \dots a_{\vec{r}_N}^\dagger a_{\vec{r}_1}^\dagger \dots a_{\vec{r}_N}^\dagger |a_{\vec{r}_1} b\rangle$$

$$= \sum_{j=1}^N \delta(\vec{r} - \vec{r}_j) \sum_{k \neq j}^N \delta(\vec{r}' - \vec{r}_k) |\vec{r}_1 \dots \vec{r}_N\rangle$$

$$\Rightarrow \times \int \frac{V(\vec{r}_1, \vec{r}')}{2} d^d r d^d r' \Rightarrow \text{works!}$$

