

Week 36: Operators in second quantization, computation of expectation values and Wick's theorem

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Week 36

- ▶ Topics to be covered
 1. Thursday: Second quantization, operators in second quantization and diagrammatic representation
 2. Friday: Second quantization and Wick's theorem
- ▶ Lecture Material: These slides, handwritten notes and Szabo and Ostlund sections 2.3 and 2.4.
- ▶ Third exercise set

Second quantization, brief summary from week 35

We can summarize our findings from last week as

$$\{a_{\alpha}^{\dagger}, a_{\beta}\} = \delta_{\alpha\beta} \quad (1)$$

with $\delta_{\alpha\beta}$ is the Kroenecker δ -symbol.

Properties of operators

The properties of the creation and annihilation operators can be summarized as (for fermions)

$$a_{\alpha}^{\dagger}|0\rangle \equiv |\alpha\rangle,$$

and

$$a_{\alpha}^{\dagger}|\alpha_1 \dots \alpha_n\rangle_{AS} \equiv |\alpha \alpha_1 \dots \alpha_n\rangle_{AS}.$$

from which follows

$$|\alpha_1 \dots \alpha_n\rangle_{AS} = a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} \dots a_{\alpha_n}^{\dagger} |0\rangle.$$

Hermitian conjugate

The hermitian conjugate has the following properties

$$a_{\alpha} = (a_{\alpha}^{\dagger})^{\dagger}.$$

Finally we found

$$a_{\alpha} \underbrace{|\alpha'_1 \alpha'_2 \dots \alpha'_{n+1}\rangle}_{\neq \alpha} = 0, \quad \text{in particular } a_{\alpha} |0\rangle = 0,$$

and

$$a_{\alpha} |\alpha \alpha_1 \alpha_2 \dots \alpha_n\rangle = |\alpha_1 \alpha_2 \dots \alpha_n\rangle,$$

and the corresponding commutator algebra

$$\{a_{\alpha}^{\dagger}, a_{\beta}^{\dagger}\} = \{a_{\alpha}, a_{\beta}\} = 0 \quad \{a_{\alpha}^{\dagger}, a_{\beta}\} = \delta_{\alpha\beta}.$$

One-body operators in second quantization

A very useful operator is the so-called number-operator. Most physics cases we will study in this text conserve the total number of particles. The number operator is therefore a useful quantity which allows us to test that our many-body formalism conserves the number of particles. In for example (d, p) or (p, d) reactions it is important to be able to describe quantum mechanical states where particles get added or removed. A creation operator a_{α}^{\dagger} adds one particle to the single-particle state α of a give many-body state vector, while an annihilation operator a_{α} removes a particle from a single-particle state α .

Getting started

Let us consider an operator proportional with $a_{\alpha}^{\dagger}a_{\beta}$ and $\alpha = \beta$. It acts on an n -particle state resulting in

$$a_{\alpha}^{\dagger}a_{\alpha}|\alpha_1\alpha_2\ldots\alpha_n\rangle = \begin{cases} 0 & \alpha \notin \{\alpha_i\} \\ |\alpha_1\alpha_2\ldots\alpha_n\rangle & \alpha \in \{\alpha_i\} \end{cases} \quad (2)$$

Summing over all possible one-particle states we arrive at

$$\left(\sum_{\alpha} a_{\alpha}^{\dagger}a_{\alpha}\right)|\alpha_1\alpha_2\ldots\alpha_n\rangle = n|\alpha_1\alpha_2\ldots\alpha_n\rangle \quad (3)$$

The number operator

The operator

$$\hat{N} = \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} \quad (4)$$

is called the number operator since it counts the number of particles in a give state vector when it acts on the different single-particle states. It acts on one single-particle state at the time and falls therefore under category one-body operators. Next we look at another important one-body operator, namely \hat{H}_0 and study its operator form in the occupation number representation.

Preserving the number of particles

We want to obtain an expression for a one-body operator which conserves the number of particles. Here we study the one-body operator for the kinetic energy plus an eventual external one-body potential. The action of this operator on a particular n -body state with its pertinent expectation value has already been studied in coordinate space. In coordinate space the operator reads

$$\hat{H}_0 = \sum_i \hat{h}_0(x_i) \quad (5)$$

and the anti-symmetric n -particle Slater determinant is defined as

$$\Phi(x_1, x_2, \dots, x_n, \alpha_1, \alpha_2, \dots, \alpha_n) = \frac{1}{\sqrt{n!}} \sum_p (-1)^p \hat{P} \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha_n}(x_n)$$

One-body operator in second quantization

Defining

$$\hat{h}_0(x_i)\psi_{\alpha_i}(x_i) = \sum_{\alpha'_k} \psi_{\alpha'_k}(x_i) \langle \alpha'_k | \hat{h}_0 | \alpha_k \rangle \quad (6)$$

we can easily evaluate the action of \hat{H}_0 on each product of one-particle functions in Slater determinant. From Eq. (6) we obtain the following result without permuting any particle pair

$$\begin{aligned} & \left(\sum_i \hat{h}_0(x_i) \right) \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\ = & \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle \psi_{\alpha'_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\ + & \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle \psi_{\alpha_1}(x_1) \psi_{\alpha'_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\ + & \dots \\ + & \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha'_n}(x_n) \end{aligned} \quad (7)$$

Interchange particles 1 and 2

If we interchange particles 1 and 2 we obtain

$$\begin{aligned} & \left(\sum_i \hat{h}_0(x_i) \right) \psi_{\alpha_1}(x_2) \psi_{\alpha_1}(x_2) \dots \psi_{\alpha_n}(x_n) \\ = & \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle \psi_{\alpha_1}(x_2) \psi_{\alpha'_2}(x_1) \dots \psi_{\alpha_n}(x_n) \\ + & \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle \psi_{\alpha'_1}(x_2) \psi_{\alpha_2}(x_1) \dots \psi_{\alpha_n}(x_n) \\ + & \dots \\ + & \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle \psi_{\alpha_1}(x_2) \psi_{\alpha_1}(x_2) \dots \psi_{\alpha'_n}(x_n) \end{aligned} \quad (8)$$

Including all possible permutations

We can continue by computing all possible permutations. We rewrite also our Slater determinant in its second quantized form and skip the dependence on the quantum numbers x_i . Summing up all contributions and taking care of all phases $(-1)^p$ we arrive at

$$\begin{aligned}\hat{H}_0|\alpha_1, \alpha_2, \dots, \alpha_n\rangle = & \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle |\alpha'_1 \alpha_2 \dots \alpha_n\rangle \\ & + \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle |\alpha_1 \alpha'_2 \dots \alpha_n\rangle \\ & + \dots \\ & + \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle |\alpha_1 \alpha_2 \dots \alpha'_n\rangle \quad (9)\end{aligned}$$

More operations

In Eq. (9) we have expressed the action of the one-body operator of Eq. (5) on the n -body state in its second quantized form. This equation can be further manipulated if we use the properties of the creation and annihilation operator on each primed quantum number, that is

$$|\alpha_1 \alpha_2 \dots \alpha'_k \dots \alpha_n\rangle = a_{\alpha'_k}^\dagger a_{\alpha_k} |\alpha_1 \alpha_2 \dots \alpha_k \dots \alpha_n\rangle \quad (10)$$

Inserting this in the right-hand side of Eq. (9) results in

$$\begin{aligned} \hat{H}_0 |\alpha_1 \alpha_2 \dots \alpha_n\rangle &= \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle a_{\alpha'_1}^\dagger a_{\alpha_1} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\ &+ \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle a_{\alpha'_2}^\dagger a_{\alpha_2} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\ &+ \dots \\ &+ \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle a_{\alpha'_n}^\dagger a_{\alpha_n} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\ &= \sum_{\alpha \beta} \langle \alpha | \hat{h}_0 | \beta \rangle a_\alpha^\dagger a_\beta |\alpha_1 \alpha_2 \dots \alpha_n\rangle \quad (11) \end{aligned}$$

Final expression for the one-body operator

In the number occupation representation or second quantization we get the following expression for a one-body operator which conserves the number of particles

$$\hat{H}_0 = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle a_{\alpha}^{\dagger} a_{\beta} \quad (12)$$

Obviously, \hat{H}_0 can be replaced by any other one-body operator which preserved the number of particles. The structure of the operator is therefore not limited to say the kinetic or single-particle energy only.

The operator \hat{H}_0 takes a particle from the single-particle state β to the single-particle state α with a probability for the transition given by the expectation value $\langle \alpha | \hat{h}_0 | \beta \rangle$.

Applying the new expression

It is instructive to verify Eq. (12) by computing the expectation value of \hat{H}_0 between two single-particle states

$$\langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle \langle 0 | a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_2}^{\dagger} | 0 \rangle \quad (13)$$

Explicit results

Using the commutation relations for the creation and annihilation operators we have

$$a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_2}^{\dagger} = (\delta_{\alpha\alpha_1} - a_{\alpha}^{\dagger} a_{\alpha_1})(\delta_{\beta\alpha_2} - a_{\alpha_2}^{\dagger} a_{\beta}), \quad (14)$$

which results in

$$\langle 0 | a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_2}^{\dagger} | 0 \rangle = \delta_{\alpha\alpha_1} \delta_{\beta\alpha_2} \quad (15)$$

and

$$\langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle \delta_{\alpha\alpha_1} \delta_{\beta\alpha_2} = \langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle \quad (16)$$

Two-body operators in second quantization

Let us now derive the expression for our two-body interaction part, which also conserves the number of particles. We can proceed in exactly the same way as for the one-body operator. In the coordinate representation our two-body interaction part takes the following expression

$$\hat{H}_I = \sum_{i < j} V(x_i, x_j) \quad (17)$$

where the summation runs over distinct pairs. The term V can be an interaction model for the nucleon-nucleon interaction or the interaction between two electrons. It can also include additional two-body interaction terms.

The action of this operator on a product of two single-particle functions is defined as

$$V(x_i, x_j) \psi_{\alpha_k}(x_i) \psi_{\alpha_l}(x_j) = \sum_{\alpha'_k \alpha'_l} \psi'_{\alpha'_k}(x_i) \psi'_{\alpha'_l}(x_j) \langle \alpha'_k \alpha'_l | \hat{V} | \alpha_k \alpha_l \rangle \quad (18)$$

More operations

We can now let \hat{H}_I act on all terms in the linear combination for $|\alpha_1 \alpha_2 \dots \alpha_n\rangle$. Without any permutations we have

$$\begin{aligned}
 & \left(\sum_{i < j} V(x_i, x_j) \right) \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\
 = & \sum_{\alpha'_1 \alpha'_2} \langle \alpha'_1 \alpha'_2 | \hat{V} | \alpha_1 \alpha_2 \rangle \psi'_{\alpha'_1}(x_1) \psi'_{\alpha'_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\
 + & \dots \\
 + & \sum_{\alpha'_1 \alpha'_n} \langle \alpha'_1 \alpha'_n | \hat{V} | \alpha_1 \alpha_n \rangle \psi'_{\alpha'_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi'_{\alpha'_n}(x_n) \\
 + & \dots \\
 + & \sum_{\alpha'_2 \alpha'_n} \langle \alpha'_2 \alpha'_n | \hat{V} | \alpha_2 \alpha_n \rangle \psi_{\alpha_1}(x_1) \psi'_{\alpha'_2}(x_2) \dots \psi'_{\alpha'_n}(x_n) \\
 + & \dots \quad (19)
 \end{aligned}$$

where on the rhs we have a term for each distinct pairs.

For the other terms on the rhs we obtain similar expressions and

Wick's theorem

The proof and derivation will be given by the whiteboard notes for week 36