Normal Order

Normal order

From Wikipedia, the free encyclopedia

For the evaluation strategy, see Normal order evaluation.

When a quantum mechanical Hamiltonian is written in **normal order**, it means that all creation operators are placed to the left of all annihilation operators in the expression. The process of putting a Hamiltonian into normal order is callled **normal ordering**. The terms **antinormal order** and **antinormal ordering** are analogously defined, where the annihilation operators are placed to the left of the creation operators.

When quantizing a classical Hamiltonian there is some freedom when choosing the operator order, and these choices lead to differences in the ground state energy.

http://books.nap.edu/html/biomems/gwick.html

Gian-Carlo Wick made many fundamental contributions to nuclear and particle physics from the 1930s, when he was a close associate of Enrico Fermi in Rome, to the 1970s, when he worked with Tsung Dao Lee at Columbia. His landmark paper, entitled "Evaluation of the collision matrix" (1950), shows how to conduct explicit practical calculations starting from the formal relations of relativistic quantum field theory through expression of the chronological product of quantum fields in terms ofa sum of normal products.

Wick's Theorem (again, see Jacek's notes)

Wick's Theorem for expectation values of operators

Consider an operator $\hat{A}$ and a wave function $|\Psi\rangle$

There always exists a decomposition:

$$\hat{A} = \hat{A}_0 + \hat{A}_+ + \hat{A}_-$$

where

$$\begin{aligned} &1^\circ \quad \hat{A}_0 = \text{const.} \\ &2^\circ \quad \hat{A}_- |\Psi\rangle = 0, \\ &3^\circ \quad \langle\Psi| \hat{A}_+ = 0. \end{aligned}$$

To demonstrate it, we introduce the projection operator:

$$\hat{P} \equiv |\Psi\rangle\langle\Psi|$$

In terms of this operator, the above decomposition can be written as:

$$\begin{aligned} \hat{A}_0 &= \langle\Psi|\hat{A}|\Psi\rangle \\ \hat{A}_- &= \left(\hat{A} - \langle\Psi|\hat{A}|\Psi\rangle\right)(1 - \hat{P}) \\ \hat{A}_+ &= (1 - \hat{P})\hat{A}\hat{P} \end{aligned}$$

Let us now calculate an expectation value of of a product of two operators:

$$\begin{aligned}\langle\Psi|\hat{A}\hat{B}|\Psi\rangle &= \langle\Psi|(\hat{A}_0+\hat{A}_+ +\hat{A}_-)(\hat{B}_0+\hat{B}_+ +\hat{B}_-)|\Psi\rangle \\ &= \hat{A}_0\hat{B}_0 + \langle\Psi|\hat{A}_-\hat{B}_+|\Psi\rangle\end{aligned}$$

or

$$\langle\Psi|\hat{A}\hat{B}|\Psi\rangle = \langle\Psi|\hat{A}|\Psi\rangle\langle\Psi|\hat{B}|\Psi\rangle + \langle\Psi|\hat{A}_-\hat{B}_+|\Psi\rangle$$

An average of a product

A product of averages

A "trouble" term

$$\begin{aligned}\langle\Psi|\hat{A}_-\hat{B}_+|\Psi\rangle &= \langle\Psi|\hat{A}_-\hat{B}|\Psi\rangle &&= \langle\Psi|\hat{A}\hat{B}_+|\Psi\rangle \\ &= \langle\Psi|\{\hat{A}_-,\hat{B}_+\}|\Psi\rangle &&= \langle\Psi|\{\hat{A}_-,\hat{B}\}|\Psi\rangle &&= \langle\Psi|\{\hat{A},\hat{B}_+\}|\Psi\rangle \\ &= \langle\Psi|[\hat{A}_-,\hat{B}_+]|\Psi\rangle &&= \langle\Psi|[\hat{A}_-,\hat{B}]|\Psi\rangle &&= \langle\Psi|[\hat{A},\hat{B}_+]|\Psi\rangle.\end{aligned}$$

Useful when dealing with fermions

Useful when dealing with bosons

How to calculate the product of many operators?

$$\langle\Psi|\hat{A}_1\hat{A}_2\ldots\hat{A}_n|\Psi\rangle$$

$$\langle\Psi|\hat{A}_1\hat{A}_2\ldots\hat{A}_n|\Psi\rangle$$
$$= \langle\Psi|\hat{A}_1|\Psi\rangle\langle\Psi|\hat{A}_2\ldots\hat{A}_n|\Psi\rangle + \langle\Psi|\hat{A}_1\_\hat{A}_2\ldots\hat{A}_n|\Psi\rangle$$

Let us introduce **the contraction:**

$$\overbrace{\hat{A}\hat{B}} \equiv \hat{A}\_\hat{B} - c\hat{B}\hat{A}\_$$

constant

For *c*=-1 (+1), contraction becomes an anticommutator (commutator)

It is also convenient to introduce **the self-contraction:**

$$\overbrace{\hat{A}} \equiv \hat{A}_0 \qquad \text{or} \qquad \overbrace{\hat{A}} = \langle\Psi|\hat{A}|\Psi\rangle$$

Why is contraction useful?

$$\langle\Psi|\hat{A}_1\hat{A}_2\hat{A}_3\ldots\hat{A}_n|\Psi\rangle = \overbrace{\hat{A}_1}\langle\Psi|\hat{A}_2\hat{A}_3\ldots\hat{A}_n|\Psi\rangle + \langle\Psi|\overbrace{\hat{A}_1\hat{A}_2}\hat{A}_3\ldots\hat{A}_n|\Psi\rangle$$
$$+c\langle\Psi|\hat{A}_2\overbrace{\hat{A}_1\hat{A}_3}\ldots\hat{A}_n|\Psi\rangle + \ldots + c^{n-2}\langle\Psi|\hat{A}_2\hat{A}_3\ldots\overbrace{\hat{A}_1\hat{A}_n}|\Psi\rangle,$$

Are we breaking the First Weinberg's Law of Progress in Theoretical Physics ?

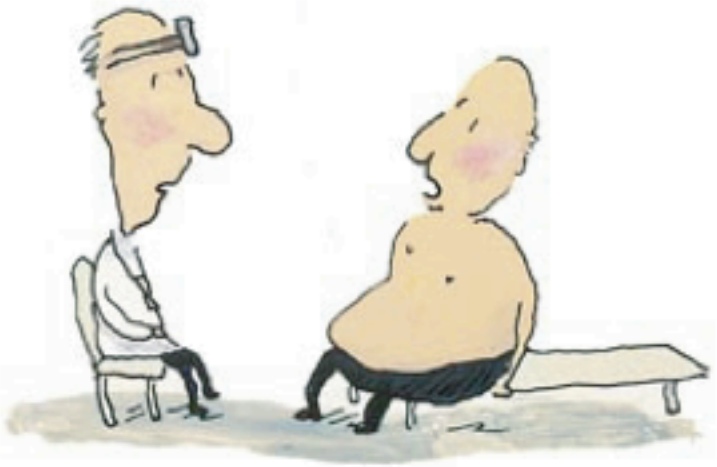
Weinberg's Laws of Progress in Theoretical Physics

From: "Asymptotic Realms of Physics" (ed. by Guth, Huang, Jaffe, MIT Press, 1983)

First Law: "The conservation of Information" (*You will get nowhere by churning equations*)

Second Law: "Do not trust arguments based on the lowest order of perturbation theory"

Third Law: "You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"



Patient: Doctor, doctor, it hurts when I do this!
Doctor: Then don't do that.

It is important to recall that the operation of contraction explicitly depends on the state (as it involves $\hat{A}$)

If all contractions are numbers, the average value becomes:

$$\langle\Phi|\hat{A}_1\hat{A}_2\hat{A}_3\ldots\hat{A}_n|\Phi\rangle = \overbrace{\hat{A}_1}\langle\Phi|\hat{A}_2\hat{A}_3\ldots\hat{A}_n|\Phi\rangle + \overbrace{\hat{A}_1\hat{A}_2}\langle\Phi|\hat{A}_3\ldots\hat{A}_n|\Phi\rangle$$
$$+c\overbrace{\hat{A}_1\hat{A}_3}\langle\Phi|\hat{A}_2\ldots\hat{A}_n|\Phi\rangle + \ldots + c^{n-2}\overbrace{\hat{A}_1\hat{A}_n}\langle\Phi|\hat{A}_2\hat{A}_3\ldots|\Phi\rangle,$$

i.e., the average of a product of operators is expressed in terms of products of averages involving less operators. The condition that all contractions are numbers is only fulfilled for certain classes of states $|\Phi\rangle$

Such states are called **product states.**

> Many-body product states are such states in which all contractions of creation and annihilation operators are numbers.

By applying the above recurrence relation, one can formulate the **Wick's theorem:**

> If all the contractions of operators appearing in the product are numbers, then the average of the product becomes a linear combination of products of all possible contractions and self-contractions.

The coefficients appearing in this linear combination are various powers of *c*.

Let us introduce

$$\overbrace{\hat{A}\hat{D}_1\hat{D}_2\ldots\hat{D}_k\hat{B}} \equiv c^k \overbrace{\hat{A}\hat{B}}\hat{D}_1\hat{D}_2\ldots\hat{D}_k$$

Using this definition, the expression for the average value of a product, becomes

$$\langle\Phi|\hat{A}_1\hat{A}_2\hat{A}_3\ldots\hat{A}_n|\Phi\rangle = \overbrace{\hat{A}_1}\langle\Phi|\hat{A}_2\hat{A}_3\ldots\hat{A}_n|\Phi\rangle + \langle\Phi|\overbrace{\hat{A}_1\hat{A}_2}\hat{A}_3\ldots\hat{A}_n|\Phi\rangle$$
$$+\langle\Phi|\overbrace{\hat{A}_1\hat{A}_2\hat{A}_3}\ldots\hat{A}_n|\Phi\rangle + \ldots + \langle\Phi|\overbrace{\hat{A}_1\hat{A}_2\hat{A}_3\ldots\hat{A}_n}|\Phi\rangle.$$

The coefficient c^k is given by a number of permutations needed to bring the two operators next to each other. In order to calculate the average value of a product, we need to calculate all possible pairwise contractions. Note that for the product states;

$$\overbrace{\hat{A}\hat{B}} = \hat{A}_-\hat{B} - c\hat{B}\hat{A}_- = \langle\Phi|\hat{A}_-\hat{B} - c\hat{B}\hat{A}_-|\Phi\rangle = \langle\Phi|\hat{A}_-\hat{B}|\Phi\rangle$$

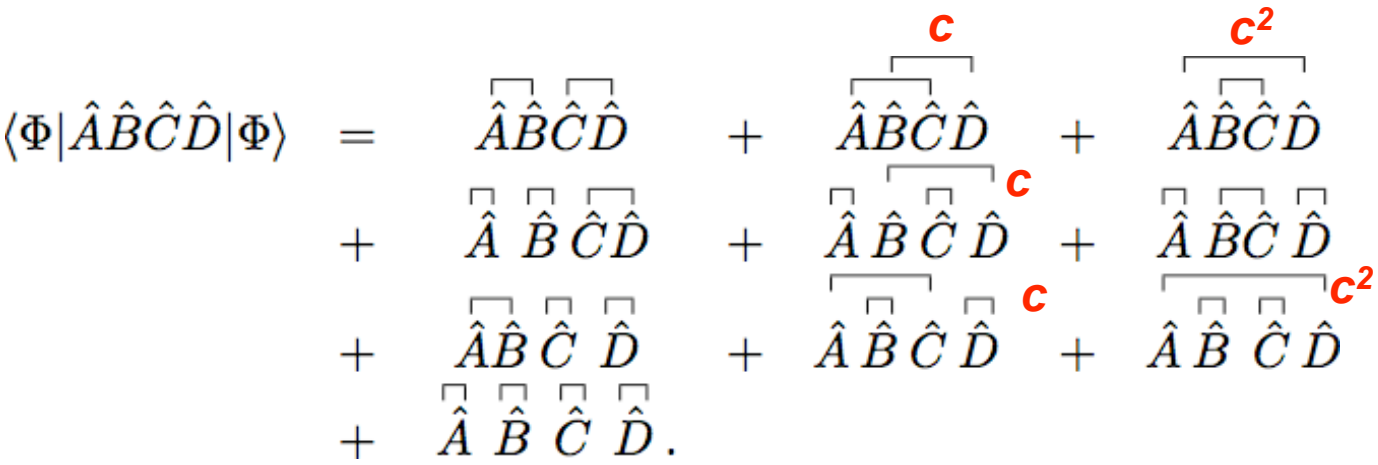
That is

$$\overbrace{\hat{A}\hat{B}} = \langle\Phi|\hat{A}\hat{B}|\Phi\rangle - \langle\Phi|\hat{A}|\Phi\rangle\langle\Phi|\hat{B}|\Phi\rangle$$

Deviation of a product average from the product of averages

In practice, we do not need the annihilating part A_-

Example: product of four operators:



$$\langle\Phi|\hat{A}\hat{B}\hat{C}\hat{D}|\Phi\rangle = \hat{A}\hat{B}\hat{C}\hat{D} + \hat{A}\hat{B}\hat{C}\hat{D} + \hat{A}\hat{B}\hat{C}\hat{D} + \hat{A}\,\hat{B}\,\hat{C}\hat{D} + \hat{A}\,\hat{B}\,\hat{C}\,\hat{D} + \hat{A}\,\hat{B}\hat{C}\,\hat{D} + \hat{A}\hat{B}\,\hat{C}\,\hat{D} + \hat{A}\,\hat{B}\,\hat{C}\,\hat{D} + \hat{A}\,\hat{B}\,\hat{C}\,\hat{D}\,.$$

$$\begin{aligned}\langle\Phi|\hat{A}\hat{B}\hat{C}\hat{D}|\Phi\rangle = \\ =&\langle\Phi|\hat{A}\hat{B}|\Phi\rangle\langle\Phi|\hat{C}\hat{D}|\Phi\rangle + c\langle\Phi|\hat{A}\hat{C}|\Phi\rangle\langle\Phi|\hat{B}\hat{D}|\Phi\rangle + \langle\Phi|\hat{A}\hat{D}|\Phi\rangle\langle\Phi|\hat{B}\hat{C}|\Phi\rangle \\ &-(1+c)\langle\Phi|\hat{A}|\Phi\rangle\langle\Phi|\hat{B}|\Phi\rangle\langle\Phi|\hat{C}|\Phi\rangle\langle\Phi|\hat{D}|\Phi\rangle.\end{aligned}$$

this term vanishes for Fermions!

Wick's theorem for Slater determinants

$$|\Phi\rangle = a^+_{\mu_1} \dots a^+_{\mu_A} |0\rangle$$

$$a_{\mu_0} = 0 \quad (\langle\Phi|a_\mu|\Phi\rangle = 0)$$

$$a_{\mu_-} = \begin{cases} 0 & \text{for} \quad \mu \in \{\mu_i\}, \\ a_\mu & \text{for} \quad \mu \notin \{\mu_i\} \end{cases}$$

$$a_{\mu_+} = \begin{cases} a_\mu & \text{for} \quad \mu \in \{\mu_i\}, \\ 0 & \text{for} \quad \mu \notin \{\mu_i\} \end{cases}$$

$$a^+_{\mu_0} = 0$$

$$a^+_{\mu_-} = \begin{cases} a^+_\mu & \text{for} \quad \mu \in \{\mu_i\}, \\ 0 & \text{for} \quad \mu \notin \{\mu_i\} \end{cases}$$

$$a^+_{\mu_+} = \begin{cases} 0 & \text{for} \quad \mu \in \{\mu_i\}, \\ a^+_\mu & \text{for} \quad \mu \notin \{\mu_i\} \end{cases}$$

Of course, in this case *c=-1.*

Let us now calculate simple contractions:

$$\overbrace{a_\mu^+ a_\nu} = \sum_{i=1}^{A} \delta_{\mu\mu_i}\delta_{\nu\mu_i},$$

$$\overbrace{a_\mu a_\nu^+} = \sum_{i=A+1}^{M} \delta_{\mu\mu_i}\delta_{\nu\mu_i},$$

$$\overbrace{a_\mu^+ a_\nu^+} = \overbrace{a_\mu a_\nu} = 0,$$

$$\overbrace{a_\mu^+} = \overbrace{a_\mu} = 0.$$

What if Slated determinant is expressed in another basis?

$$|\Phi'\rangle = a'^{+}_{\mu_1} \dots a'^{+}_{\mu_A} |0\rangle$$

$$a'^{+}_{\mu} = \sum_{\nu} U_{\mu\nu} a^{+}_{\nu}$$

$$a_{\mu_0} = 0$$

$$a_{\mu_-} = \sum_{\nu \notin \{\mu_i\}} U^{T}_{\mu\nu} a'_{\nu} = \sum_{i=A+1}^{M} \sum_{\nu} U^{T}_{\mu\nu_i} U^{*}_{\nu_i\nu} a_{\nu},$$

$$a_{\mu_+} = \sum_{\nu \in \{\mu_i\}} U^{T}_{\mu\nu} a'_{\nu} = \sum_{i=1}^{A} \sum_{\nu} U^{T}_{\mu\nu_i} U^{*}_{\nu_i\nu} a_{\nu}$$

$$a^{+}_{\mu_0} = 0$$

$$a^{+}_{\mu_-} = \sum_{\nu \in \{\mu_i\}} U^{+}_{\mu\nu} a'^{+}_{\nu} = \sum_{i=1}^{A} \sum_{\nu} U^{+}_{\mu\nu_i} U_{\nu_i\nu} a^{+}_{\nu},$$

$$a^{+}_{\mu_+} = \sum_{\nu \notin \{\mu_i\}} U^{+}_{\mu\nu} a'^{+}_{\nu} = \sum_{i=A+1}^{M} \sum_{\nu} U^{+}_{\mu\nu_i} U_{\nu_i\nu} a^{+}_{\nu},$$

$$\overbrace{a_\mu^+ a_\nu} = \sum_{i=1}^{A} U^+_{\mu\nu_i} U_{\nu_i\nu},$$

$$\overbrace{a_\mu a_\nu^+} = \sum_{i=A+1}^{M} U^T_{\mu\nu_i} U^*_{\nu_i\nu},$$

$$\overbrace{a_\mu^+ a_\nu^+} = \overbrace{a_\mu a_\nu} = 0,$$

… and all self-contractions vanish!