5. WICK'S THEOREM

Main idea : reduce arbitrary products of creation and annihilation operators into sums of products of pairs of operators.

Formulated by Gian Carlo Wick (Italian physicist) in 1950.
There exist many variants (time-dependent, off diagonal, generalised, ...) here we will study its simplest version (time-independent).

Vacuum state

Given a complete set of creation and annihilation operators c_α^+ and c_α obeying anticommutation relations, there exist a corresponding vacuum state $|\phi_0\rangle$ such that

$$c_\alpha |\phi_0\rangle = 0 \qquad \forall \alpha$$

For example

I) particle vacuum

a_α^+ and a_α standard particle creation / annihilation operators

$$\Rightarrow \quad |\phi_0\rangle = |0\rangle \qquad \text{and} \qquad a_\alpha |0\rangle = 0 \qquad \forall \alpha$$

II) Fermi vacuum

Slater determinant $|\phi_0\rangle = |\phi\rangle \equiv \prod_{\alpha=1}^{N} a_\alpha^+ |0\rangle$

Is there a set of annihilation operators for which it is the vacuum?

$$b_\alpha = \begin{cases} a^\dagger_\alpha & \text{for } \alpha = 1, \dots, N \quad \text{(occupied states in } |\Phi_0\rangle) \\ a_\alpha & \text{for } \alpha = N+1, \dots \quad \text{(unoccupied states in } |\Phi_0\rangle) \end{cases}$$

iii) generic vacuum

One can introduce a set of b_α and $b^\dagger_\alpha$ that are linear combinations of a_α and $a_\alpha^\dagger$.

Then in general $b_\alpha |0\rangle \neq 0$, but again one can find a corresponding vacuum $|\Phi_0\rangle$ for which $b_\alpha |\Phi_0\rangle = 0 \quad \forall \alpha$

Normal product

→ Defined with respect to a set of creation and annihilation operators <u>and</u> their corresponding vacuum

$$\boxed{\text{Definition: the normal product of a starting product of creation and annihilation operators is obtained by bringing all annihilation operators to the right of all creation operators and by multiplying the result with the signature of the performed permutation.}}$$

The normal product of an operator $ABC \dots Z$ (where $A, B, \dots$ can be a creation or an annihilation operator) is denoted by

$$:ABC \dots Z:$$

For example (particle vacuum)

$$:a_\alpha a_\beta^\dagger: = -a_\beta^\dagger a_\alpha$$

$$:a_\alpha a_\beta^\dagger a_\gamma^\dagger a_\delta: = + a_\beta^\dagger a_\gamma^\dagger a_\alpha a_\delta = - a_\beta^\dagger a_\gamma^\dagger a_\delta a_\alpha$$

→ Important property: the average value of the normal product in the corresponding vacuum is zero.

$$\langle\Phi_0| :ABC \dots Z: |\Phi_0\rangle = 0$$

It trivially follows from the definition of normal product and the properties

$$\langle\Phi_0| c_\alpha^\dagger = 0$$

$$c_\alpha |\Phi_0\rangle = 0$$

→ If we take the normal product of operators with respect to a vacuum that isn't their vacuum, the result will be different than just moving annihilation operators to the right

For example consider

$$b_\mu = \frac{1}{\sqrt{2}}\left(a_\mu + a_{\bar{\mu}}^\dagger\right) \qquad \text{with} \quad \bar{\mu} \neq \mu$$

The normal product of $b_\mu b_\nu^\dagger$ with respect to the b's vacuum is

$$N[b_\mu b_\nu^\dagger] = - b_\nu^\dagger b_\mu$$

to differentiate from $: \; :$ which refers to the a's vacuum

$$= -\frac{1}{2}\left(a_\nu^\dagger + a_{\bar{\nu}}\right)\left(a_\mu + a_{\bar{\mu}}^\dagger\right)$$

$$= -\frac{1}{2}\left[a_\nu^\dagger a_\mu + a_\nu^\dagger a_{\bar\mu}^\dagger + a_{\bar\nu} a_\mu + a_{\bar\nu} a_{\bar\mu}^\dagger \right]$$

$$= -\frac{1}{2} a_\nu^\dagger a_\mu - \frac{1}{2} a_{\bar\mu}^\dagger a_\nu^\dagger - \frac{1}{2} a_\mu a_{\bar\nu} + \frac{1}{2} a_{\bar\mu}^\dagger a_{\bar\nu} - \frac{1}{2}\delta_{\bar\mu\bar\nu}$$

$$= :b_\mu b_\nu^\dagger: - \frac{1}{2}\delta_{\bar\mu\bar\nu}$$

This shows the importance of specifying the reference vacuum.

Contractions

The contraction of two operators is defined as

$$\boxed{\overline{AB} \equiv AB - :AB:}$$

→ Since it involves the normal product, the contraction also depends on a reference vacuum

→ The contraction of two operators (in their corresponding vacuum) is necessarily a number.

Only four possibilities:

$$\overline{c_\alpha^\dagger c_\beta^\dagger} = c_\alpha^\dagger c_\beta^\dagger - c_\alpha^\dagger c_\beta^\dagger = 0$$

$$\overline{c_\alpha c_\beta} = c_\alpha c_\beta - c_\alpha c_\beta = 0$$

$$\overline{c_\alpha^\dagger c_\beta} = c_\alpha^\dagger c_\beta - c_\alpha^\dagger c_\beta = 0$$

$$\overline{c_\alpha c_\beta^\dagger} = c_\alpha c_\beta^\dagger - \left(-c_\beta^\dagger c_\alpha\right) = \left\{c_\alpha, c_\beta^\dagger\right\} = \delta_{\alpha\beta}$$

→ It follows that

$$\langle \Phi_0 | \overbrace{AB} | \Phi_0 \rangle = \langle \Phi_0 | AB | \Phi_0 \rangle - \cancel{\langle \Phi_0 | :AB: | \Phi_0 \rangle}$$

just a number

$$\Rightarrow \boxed{\overbrace{AB} = \langle \Phi_0 | AB | \Phi_0 \rangle}$$

→ This property remains valid in the more general case where the reference vacuum is not the vacuum of the operators in the product. In that case, however, the four contractions

$$\overbrace{c_\alpha^+ c_\beta^+}, \quad \overbrace{c_\alpha c_\beta}, \quad \overbrace{c_\alpha^+ c_\beta}, \quad \overbrace{c_\alpha c_\beta^+}$$

will give something more complicated than 0 and $\delta_{\alpha\beta}$.

An interesting case (of relevance for the following) is when $|\Phi_0\rangle$ is a Slater determinant

$$|\Phi_0\rangle = \prod_{\alpha=1}^{N} a_\alpha^+ |0\rangle$$

and the operators are given is some other basis $\{b_\lambda^+\}$

Then

$$\overbrace{b_\alpha^+ b_\beta^+} = \langle \Phi_0 | b_\alpha^+ b_\beta^+ | \Phi_0 \rangle = 0$$

$$\overbrace{b_\alpha b_\beta} = \langle \Phi_0 | b_\alpha b_\beta | \Phi_0 \rangle = 0$$

$$\overbrace{b_\alpha^+ b_\beta} = \langle \Phi_0 | b_\alpha^+ b_\beta | \Phi_0 \rangle \equiv \rho_{\beta\alpha}$$ density matrix

$$\overbrace{b_\alpha b_\beta^+} = \langle \Phi_0 | b_\alpha b_\beta^+ | \Phi_0 \rangle \equiv \delta_{\alpha\beta} - \rho_{\alpha\beta}$$

Let us introduce one more definition: a normal product with contractions is

$$\contraction{:ABC\ldots}{R}{\ldots S\ldots}{T}\contraction[2ex]{:ABC\ldots R\ldots}{S}{\ldots T\ldots}{U}:ABC\ldots R\ldots S\ldots T\ldots U\ldots: \;=\; (-1)^N \,\contraction{}{R}{}{T}RT\,\contraction{}{S}{}{U}SU\ldots \;:ABC\ldots:$$

where all the contracted pairs have been put in front of the normal product and the signature of the corresponding permutation appears.

Motivation for Wick's theorem

Consider the following example (typical problem of interest): we have

i) a first Slater determinant $|\alpha\beta\ldots\rangle$

ii) a second Slater determinant in which α has been emptied and μ occupied, $|\mu\beta\ldots\rangle$

iii) a one-body operator F and a two-body operator G

and want to compute

$$\langle\alpha\beta\ldots|\,F\,G\,|\mu\beta\ldots\rangle$$

- In first quantisation one has to expand both $|\alpha\beta\ldots\rangle$ and $|\mu\beta\ldots\rangle$ in terms of direct-product states and act with F and G $\rightarrow$ gives rise to $(N!)^2$ terms to deal with!

- In second quantisation one can take the first Slater determinant as a reference

$$|\Phi\rangle = \prod_{\alpha=1}^{N} a^{+}_{\alpha}|0\rangle$$

and rewrite the second one as

$$|\Phi^{\mu}_{\alpha}\rangle \equiv a^{+}_{\mu} a_{\alpha} |\Phi\rangle$$

"particle-hole" excitation

Then (expressing F and G in the basis $\{a^{+}_{\alpha}\}$)

$$\langle\alpha\beta\ldots|FG|\mu\beta\ldots\rangle = \langle\Phi|FG|\Phi^{\mu}_{\alpha}\rangle$$

$$= \sum_{\beta\gamma} \frac{1}{2}\sum_{\lambda\nu\delta\varepsilon} f_{\beta\gamma}\, g_{\lambda\nu\delta\varepsilon} \langle\Phi|a^{+}_{\beta} a_{\gamma}\, a^{+}_{\lambda} a^{+}_{\nu} a_{\varepsilon} a_{\delta}\, a^{+}_{\mu} a_{\alpha}|\Phi\rangle$$

$\downarrow$

two options:

i) work out all permutations explicitly

ii) ... Wick's theorem

Wick's theorem

"A product of a string of creation and annihilation operators is equal to their normal product plus the sum of all possible normal products with contractions!"

In formulae

$$
\begin{aligned}
ABCD\ldots YZ = {} & :ABCD\ldots YZ: \\
& + :\contraction{}{A}{}{B}AB\,CD\ldots YZ: + :\contraction{}{A}{B}{C}ABCD\ldots YZ: + \ldots \\
& + :A\contraction{}{B}{}{C}BCD\ldots YZ: + :A\contraction{}{B}{C}{D}BCD\ldots YZ: + \ldots \\
& + \ldots \\
& + :\contraction{}{A}{}{B}AB\contraction{}{C}{}{D}CD\ldots YZ: + :\contraction{}{A}{B}{C}\contraction[2ex]{A}{B}{C}{D}ABCD\ldots YZ: + \ldots \\
& + \ldots \\
& + :\contraction{}{A}{}{B}AB\contraction{}{C}{}{D}CD\ldots \contraction{}{Y}{}{Z}YZ: + :\contraction{}{A}{B}{C}\contraction[2ex]{A}{B}{C}{D}ABCD\ldots \contraction{}{Y}{}{Z}YZ: + \ldots
\end{aligned}
$$

→ Important property: taking the vacuum expectation value of both sides one has

$$
\begin{aligned}
\langle \phi_0 | ABCD\ldots YZ | \phi_0 \rangle = {} & \contraction{}{A}{}{B}AB\contraction{}{C}{}{D}CD\ldots\contraction{}{Y}{}{Z}YZ \\
& - \contraction{}{A}{}{C}AC\contraction{}{B}{}{D}BD\ldots\contraction{}{Y}{}{Z}YZ \\
& + \contraction{}{A}{}{D}AD\contraction{}{B}{}{C}BC\ldots\contraction{}{Y}{}{Z}YZ \\
& + \ldots
\end{aligned}
$$

i.e. the sum of all fully contracted terms.

→ Remark: Wick's theorem is simply a rewriting of the original operator. As it employs normal products, however, a reference vacuum is associated to this rewriting. This vacuum impacts the evaluation of the actual result.

→ Outline of proof of Wick's theorem

In a normal-ordered product all contractions vanish because there cannot be a $\overline{a_\alpha a_\beta^\dagger}$ contraction (all others are zero)

Then if a string of operators is already in a normal-ordered form one can write

$$a_\alpha^\dagger a_\beta^\dagger \cdots a_\mu a_\nu = :a_\alpha^\dagger a_\beta^\dagger \cdots a_\mu a_\nu:$$

$$= :a_\alpha^\dagger a_\beta^\dagger \cdots a_\mu a_\nu: + \text{sum of all possible normal orders with contractions}$$

(that vanish)

If there is one annihilation operator on the left of a creation operator

$$a_\alpha^\dagger a_\beta^\dagger \cdots a_\lambda a_\delta^\dagger \cdots a_\mu a_\nu$$

$$= a_\alpha^\dagger a_\beta^\dagger \cdots \left[\{a_\lambda, a_\delta^\dagger\} - a_\delta^\dagger a_\lambda \right] \cdots a_\mu a_\nu$$

$$= a_\alpha^\dagger a_\beta^\dagger \cdots \delta_{\lambda\delta} \cdots a_\mu a_\nu - a_\alpha^\dagger a_\beta^\dagger \cdots a_\delta^\dagger a_\lambda \cdots a_\mu a_\nu$$

$$= :a_\alpha^\dagger a_\beta^\dagger \cdots \overline{a_\lambda a_\delta^\dagger} \cdots a_\mu a_\nu: + :a_\alpha^\dagger a_\beta^\dagger \cdots a_\lambda a_\delta^\dagger \cdots a_\mu a_\nu:$$

+ sum of all other possible normal orders with contractions (that vanish)

And so on ...

Examples of applications of Wick's theorem

$$a^+_\alpha a_\beta = \overline{a^+_\alpha a_\beta} + :a^+_\alpha a_\beta:$$

$$\begin{aligned}
a^+_\alpha a^+_\beta a_\delta a_\gamma = \; & :a^+_\alpha a^+_\beta a_\delta a_\gamma: \\
& + \overline{a^+_\alpha a^+_\beta} \; :a_\delta a_\gamma: && \to \text{vanishes if } |\Phi\rangle = \text{Slater} \\
& - \overline{a^+_\alpha a_\delta} \; :a^+_\beta a_\gamma: \\
& + \overline{a^+_\alpha a_\gamma} \; :a^+_\beta a_\delta: \\
& + \overline{a^+_\beta a_\delta} \; :a^+_\alpha a_\gamma: \\
& - \overline{a^+_\beta a_\gamma} \; :a^+_\alpha a_\delta: \\
& + \overline{a_\delta a_\gamma} \; :a^+_\alpha a^+_\beta: && \to \text{vanishes if } |\Phi\rangle = \text{Slater} \\
& + \overline{a^+_\alpha a^+_\beta} \; \overline{a_\delta a_\gamma} && \to \text{vanishes if } |\Phi\rangle = \text{Slater} \\
& - \overline{a^+_\alpha a_\delta} \; \overline{a^+_\beta a_\gamma} \\
& + \overline{a^+_\alpha a_\gamma} \; \overline{a^+_\beta a_\delta}
\end{aligned}$$

Application to nuclear Hamiltonian

Consider only two-body interaction for simplicity.
Written in an arbitrary basis $B_1 = \{a^+_\alpha\}$

$$H = \sum_{\alpha\beta} t_{\alpha\beta} \, a^+_\alpha a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \, a^+_\alpha a^+_\beta a_\delta a_\gamma$$

Apply Wick's theorem with respect to a Slater determinant in a (different) basis $\mathcal{B}_1' = \{ b^+_\lambda \}$

$$|\phi_0\rangle = \prod_{\lambda=1}^{N} b^+_\lambda |0\rangle$$

Then

$$H = \sum_{\alpha\beta} t_{\alpha\beta} \left(\overbracket{a^+_\alpha a_\beta} + :a^+_\alpha a_\beta: \right)$$

$$+ \frac{1}{2} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} \Big(\overbracket{a^+_\alpha a_\gamma}\, \overbracket{a^+_\beta a_\delta} - \overbracket{a^+_\alpha a_\delta}\, \overbracket{a^+_\beta a_\gamma} + \overbracket{a^+_\alpha a^+_\beta}\, \overbracket{a_\delta a_\gamma}$$

$$+ \overbracket{a^+_\alpha a_\gamma} :a^+_\beta a_\delta: - \overbracket{a^+_\alpha a_\delta} :a^+_\beta a_\gamma: - \overbracket{a^+_\beta a_\gamma} :a^+_\alpha a_\delta: + \overbracket{a^+_\beta a_\delta} :a^+_\alpha a_\gamma:$$

$$+ \overbracket{a_\delta a_\gamma} :a^+_\alpha a^+_\beta: + \overbracket{a^+_\alpha a^+_\beta} :a_\delta a_\gamma:$$

$$+ :a^+_\alpha a^+_\beta a_\delta a_\gamma: \Big) \quad (*)$$

these terms are zero if $|\phi\rangle$ has a fixed number of particles N

Introduce definition

$$\rho_{\beta\alpha} \equiv \overbracket{a^+_\alpha a_\beta} = \langle \phi_0 | a^+_\alpha a_\beta | \phi_0 \rangle$$

one-body density matrix

Property: ρ is hermitian

$$\rho^*_{\beta\alpha} = \langle \phi_0 | a^+_\alpha a_\beta | \phi_0 \rangle^* = \langle \phi_0 | (a^+_\alpha a_\beta)^\dagger | \phi_0 \rangle = \langle \phi_0 | a^+_\beta a_\alpha | \phi_0 \rangle = \rho_{\alpha\beta}$$

One can also define an <u>anomalous</u> density matrix

$$\kappa_{\alpha\beta} \equiv \overbrace{a_\alpha a_\beta} = \langle \Phi_0 | a_\alpha a_\beta | \Phi_0 \rangle$$

which is non-zero only if $|\Phi_0\rangle$ does not conserve particle number.

Property: κ is antisymmetric

$$\kappa_{\alpha\beta} = \langle \Phi_0 | a_\alpha a_\beta | \Phi_0 \rangle = \langle \Phi_0 | (-a_\beta a_\alpha) | \Phi_0 \rangle = -\kappa_{\beta\alpha}$$

With these definitions, ⊛ can be rewritten as (one has to rename the indices in some of the sums) (and omitting anomalous terms)

remember $\boxed{\bar{V}_{\alpha\beta\gamma\delta} \equiv V_{\alpha\beta\gamma\delta} - V_{\alpha\beta\delta\gamma}}$

$$H = \sum_{\alpha\beta} t_{\alpha\beta} \rho_{\beta\alpha} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \bar{V}_{\alpha\beta\gamma\delta} \rho_{\gamma\alpha} \rho_{\delta\beta} \qquad [0\text{-body}]$$

$$+ \sum_{\alpha\beta} t_{\alpha\beta} :a_\alpha^\dagger a_\beta: + \sum_{\alpha\beta\gamma\delta} \bar{V}_{\alpha\beta\gamma\delta} \rho_{\gamma\alpha} :a_\beta^\dagger a_\delta: \qquad [1\text{-body}]$$

$$+ \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{V}_{\alpha\beta\gamma\delta} :a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma: \qquad [2\text{-body}]$$

$$= H_{0B}^{NO} + H_{1B}^{NO} + H_{2B}^{NO}$$

Vacuum expectation value
$\langle \Phi_0 | H | \Phi_0 \rangle$
= energy of the reference vacuum state

one-body operator
→ easy to treat

two-body operator
→ difficult part

→ The normal-ordered one-body operator can be rewritten as

$$H_{1B}^{NO} = \sum_{\alpha\beta} h_{\alpha\beta} : a_\alpha^\dagger a_\beta :$$

where we have introduced the Hartree-Fock Hamiltonian

$$h \equiv T + U$$

with the Hartree-Fock (one-body) potential

$$U_{\alpha\beta} \equiv \sum_{\gamma\delta} \bar{V}_{\alpha\gamma\beta\delta}\, \rho_{\delta\gamma}$$

→ A one-body Hamiltonian can be usually solved exactly, while a two-body Hamiltonian is much harder.

$$H |\Psi_k\rangle = E_k |\Psi_k\rangle$$

is the full problem.

If

$$H = \sum_{i=1}^{N} h(i) \qquad \text{one-body operators only}$$

then

$$H|\Psi_k\rangle = E_k |\Psi_k\rangle \longrightarrow h|\phi_\alpha\rangle = \varepsilon_\alpha |\phi_\alpha\rangle$$

from N-body problem to N one-body problems

Strategy:

$$H = \underbrace{H^{NO}_{0B} + H^{NO}_{1B}}_{\equiv H_0} + \underbrace{H^{NO}_{2B}}_{\equiv H_1}$$

i) Solve exactly for H_0

ii) Include "residual interaction" H_1 as well as you can (e.g. in perturbation)

Generalised Wick's theorem

We motivated Wick's theorem by the computation of a matrix element of the type

normal-ordered form

$$\langle \Phi | FG | \Phi^{\mu}_{\alpha} \rangle = \langle \Phi | FG\, a^{+}_{\mu} a_{\alpha} | \Phi \rangle$$

How do we proceed if the operators FG are put in a normal-ordered form (as done for H above)?

Generalised Wick's theorem: "Apply standard Wick's theorem but omit all the terms in which at least one contraction is taken among operators belonging to the same original string of normal ordered operators."

↓

Uses the fact that any contraction from a normal product is necessarily zero.