Ch. 4: Quantum many-particle theory and quantum field theory, Wick's theorem

Ref. for 1st topic: L. I. Schiff, Quantum Mechanics, 3rd ed., § 54 and 55.

Goal: We will prove that non-rel. quantum many-particle theory is equivalent to a "second quantization" of the "classical" Schrödinger field.

This is important for 2 reasons:

a) quantum field theory (QFT) is the most fundamental theory we have (so far)

b) many calculational methods developed for QFT, e.g. Wick's theorem for quantum field operators, can be carried over to many-body theory.

In QFT, one usually starts from a classical field theory (use Lagrange / Hamilton formalism). Quantization is achieved by

quantization of field amplitudes. The "field quanta" are the "particles" we observe (e.g. photons, electrons, etc.)

We develop now the steps we need for QFT, starting from a classical field theory. Since most students are familiar with classical mechanics, we develop the theory for classical fields in parallel to the theory of classical mechanics, using the principle of least action, Lagrange & Hamilton formalism, and Poisson brackets.

$\boxed{\text{Comparison: class. mechanics} \leftrightarrow \text{class. field theory}}$

class. mechanics	class. field theory
gen. coordinates $q_i(t)$ → gen. velocities $\dot{q}_i(t)$ →	field amplitudes $\psi(\vec{r}_i, t)$ $\xrightarrow{\text{continuum}}$ $\psi(\vec{r}, t)$ $\partial\psi(\vec{r}_i, t)/\partial t$
Lagrange function $L(q_i, \dot{q}_i, t)$	Lagrange function $L = \int d^3r \, \mathcal{L}\left(\psi(\vec{r}, t), \frac{\partial\psi(\vec{r}, t)}{\partial t}, \frac{\partial\psi}{\partial x_i}, t\right)$ Lagrange density
action integral $S = \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t)\, dt$	action integral $S = \int_{t_1}^{t_2} L\, dt = \int_{t_1}^{t_2} dt \int d^3r \, \mathcal{L}$

class. mechanics	class. field theory

class. mechanics

least-action principle

$$\delta S = 0 \rightarrow \int_{t_1}^{t_2} dt\, \delta L(q_i, \dot q_i, t) = 0$$

$$\int_{t_1}^{t_2} dt \left(\frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot q_i} \delta \dot q_i \right) = 0$$

$\Rightarrow$ Lagr. equations of motion

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot q_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

Hamilton fctn

can. momentum $p_i = \dfrac{\partial L}{\partial \dot q_i}$

$$H = \sum_{i=1}^{n} p_i \dot q_i - L$$

Poisson brackets

$$F = F(q_i, p_i, t)$$

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \{F, H\}_{P.B.}$$

$$\{q_i, q_k\} = 0 = \{p_i, p_k\}$$

$$\{q_i, p_k\} = \delta_{ik}$$

class. field theory

least-action principle

$$\delta S = 0 \rightarrow \int_{t_1}^{t_2} dt \int d^3r\, \delta \mathcal{L} = 0$$

$$\int_{t_1}^{t_2} dt \int d^3r \left[\frac{\partial \mathcal{L}}{\partial \psi} \delta \psi + \frac{\partial \mathcal{L}}{\partial(\partial\psi/\partial t)} \delta\left(\frac{\partial \psi}{\partial t}\right) + \sum_{i=1}^{3} \frac{\partial \mathcal{L}}{\partial(\partial\psi/\partial x_i)} \delta\left(\frac{\partial\psi}{\partial x_i}\right) \right] = 0$$

$\Rightarrow$ Lagr. eqns for class. field $\psi(\vec r, t)$:

$$\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial(\partial\psi/\partial t)}\right) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left[\frac{\partial \mathcal{L}}{\partial(\partial\psi/\partial x_i)}\right] - \frac{\partial \mathcal{L}}{\partial \psi} = 0$$

Hamilton function

can. field momentum $\overset{\text{class}}{\pi}(\vec r, t) = \dfrac{\partial \mathcal{L}}{\partial(\partial\psi/\partial t)}$

$$H = \int d^3r\, \mathcal{H}(\psi(r,t); \pi(\vec r, t))$$

$\downarrow$ Hamilton density

$$\mathcal{H}(\psi, \pi) = \pi(\vec r, t) \cdot \dot\psi(\vec r, t) - \mathcal{L}$$

Poisson brackets

$$F = F(\psi(\vec r, t); \pi(\vec r, t))$$

$$\frac{dF(\psi,\pi)}{dt} = \frac{\partial F}{\partial t} + \{F, H\}_{P.B.}$$

$$\{\psi(\vec r, t), \psi(\vec r\,', t)\} = 0 = \{\pi(r,t), \pi(\vec r\,', t)\}$$

$$\{\psi(\vec r, t), \pi(\vec r\,', t)\} = \delta^3(\vec r - \vec r\,')$$

Field quantization

class. fields $\psi(\vec{r},t)$, $\pi(\vec{r},t)$ $\longrightarrow$ field operators $\hat{\psi}(\vec{r},t)$, $\hat{\pi}(\vec{r},t)$

Can. quantization rule for P.B.'s : $\{A,B\}_{P.B.} \rightarrow \frac{1}{i\hbar}[\hat{A},\hat{B}]_-$
where $[\,,\,]_-$ denotes the commutator.

eq. of motion of quantum field

$$\boxed{\frac{d\hat{F}(\hat{\psi},\hat{\pi})}{dt} = \frac{\partial \hat{F}(\hat{\psi},\hat{\pi})}{\partial t} + \frac{1}{i\hbar}[\hat{F},\hat{H}]_-} \tag{1}$$

For the field operators $\hat{\psi}$ and $\hat{\pi}$ themselves, we have boson commutators $[\,,\,]_-$ and fermion anticommutators $[\,,\,]_+$:

$$\boxed{\begin{aligned} &[\hat{\psi}(\vec{r},t),\hat{\psi}(\vec{r}\,',t)]_\mp = 0 = [\hat{\pi}(r,t),\hat{\pi}(\vec{r}\,',t)]_\mp \\ &[\hat{\psi}(r,t),\hat{\pi}(\vec{r}\,',t)]_\mp = i\hbar\,\delta^3(\vec{r}-\vec{r}\,') \end{aligned}} \tag{2}$$

"Classical" Schrödinger field $\psi(\vec{r},t)$

We regard the Schrödinger field $\psi(\vec{r},t)$ as a classical, complex-valued field. In fact, the Schrödinger eq. can be derived from the foll. Lagrange density ("classical")

$$\boxed{\begin{aligned} &\mathcal{L}\left(\psi,\psi^*;\frac{\partial\psi}{\partial t},\frac{\partial\psi^*}{\partial t};\nabla\psi,\nabla\psi^*;t\right) = \\ &= i\hbar\,\psi^*\frac{\partial\psi}{\partial t} - \frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi - V(\vec{r},t)\psi^*\psi \end{aligned}} \tag{3}$$

Note: Because the Schrödinger field is complex, $\psi = (\psi_1 + i\psi_2)$, we have to do two variations, either with respect to ψ_1 and ψ_2 or, equivalently, with respect to ψ and ψ^*.

Variation with respect to ψ^* yields

$$\underbrace{\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial(\partial\psi^*/\partial t)}\right)}_{=0} + \underbrace{\sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left[\frac{\partial \mathcal{L}}{\partial(\partial\psi^*/\partial x_i)}\right]}_{=-\frac{\hbar^2}{2m}\nabla^2\psi} - \underbrace{\frac{\partial \mathcal{L}}{\partial \psi^*}}_{=\left(i\hbar\frac{\partial\psi}{\partial t} - V\psi\right)} = 0$$

which yields the "classical" Schrödinger eq.

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi}$$

Variation with respect to ψ yields

$$\underbrace{\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial(\partial\psi/\partial t)}\right)}_{=i\hbar\frac{\partial\psi^*}{\partial t}} + \underbrace{\sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left[\frac{\partial \mathcal{L}}{\partial(\partial\psi/\partial x_i)}\right]}_{=-\frac{\hbar^2}{2m}\nabla^2\psi^*} - \underbrace{\frac{\partial \mathcal{L}}{\partial \psi}}_{=+V\psi^*} = 0$$

which is the c.c. of the Schrödinger equation.

canonical field momentum: $\boxed{\pi(\vec{r},t) = \frac{\partial \mathcal{L}}{\partial(\partial\psi/\partial t)} = i\hbar\psi^*(\vec{r},t)}$ (4)

Class. Hamilton density

$$\mathcal{H} = \pi\cdot\dot{\psi} - \mathcal{L} = \cancel{i\hbar\psi^*\frac{\partial\psi}{\partial t}} - \left(\cancel{i\hbar\psi^*\frac{\partial\psi}{\partial t}} - \frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi - V\psi^*\psi\right)$$

$$\mathcal{H} = +\frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi + V\psi^*\psi$$

Hamiltonian $H = \int d^3r\,\mathcal{H} = \int d^3r\left(\frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi + V\psi^*\psi\right)$

partial integr.

$$\boxed{H = \int d^3r\, \psi^*(\vec{r},t)\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right]\psi(\vec{r},t)} \quad \underline{(5)}$$

"classical"

"Second quantization" of "classical" Schrödinger field

Let's assume we have bosons. We replace the classical fields $\psi(\vec{r},t)$, $\pi(\vec{r},t)$ by the quantum field operators $\hat{\psi}(\vec{r},t)$, $\hat{\pi}(\vec{r},t)$ with the commutators (2):

$$[\hat{\psi}(\vec{r},t), \pi(\vec{r}\,',t)]_- = i\hbar\, \delta^3(\vec{r}-\vec{r}\,') \qquad \underline{(6a)}$$

Using $\pi(\vec{r}\,',t) \overset{(4)}{=} i\hbar\, \psi^*(\vec{r}\,',t) \rightarrow i\hbar\, \hat{\psi}^+(\vec{r}\,',t)$ it follows that

$$\boxed{[\hat{\psi}(\vec{r},t), \hat{\psi}^+(\vec{r}\,',t)] = \delta^3(\vec{r}-\vec{r}\,')} \qquad \underline{(6b)}$$

From the general eq. of motion (1) we obtain for $\hat{F}(\hat{\psi},\hat{\pi}) = \hat{\psi}$:

$$\frac{d\hat{\psi}(\vec{r},t)}{dt} = 0 + \frac{1}{i\hbar}[\hat{\psi}, \hat{H}]_-$$

resulting in the "<u>second-quantized</u>" <u>Hamiltonian</u>

$$\boxed{\hat{H} = \int d^3r\, \hat{\psi}^+(\vec{r},t)\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right)\hat{\psi}(\vec{r},t)} \quad \underline{(7)}$$

and the eq. of motion for $\hat{\psi}$:

$$i\hbar\, \frac{d\hat{\psi}(\vec{r},t)}{dt} = [\hat{\psi}(\vec{r},t), \hat{H}]_- =$$

$$= \left[\hat{\psi}(\underline{\underline{\vec{r}}},t), \int d^3\underline{\underline{r}}'\, \hat{\psi}^+(\underline{\underline{\vec{r}\,'}},t)\left(-\frac{\hbar^2}{2m}\underline{\underline{\nabla'}}^2 + V(\underline{\underline{\vec{r}\,'}},t)\right)\hat{\psi}(\underline{\underline{\vec{r}\,'}},t)\right]_-$$

We evaluate the commutator using the shorthand notation

$$\psi \equiv \hat{\psi}(\vec{r},t) \qquad \psi' = \psi(\vec{r}\,',t) \qquad V' = V(\vec{r}\,',t) \quad \text{etc.}$$

$$\Rightarrow [\hat{\psi}, \hat{H}]_- = [\psi, \int d^3r' \psi^{+\prime} (-\tfrac{\hbar^2}{2m} \nabla'^2 + V') \psi']_- =$$

$$= \int d^3r' \left\{ \psi \psi^{+\prime} (-\tfrac{\hbar^2}{2m} \nabla'^2 + V') \psi' - \psi^{+\prime} (-\tfrac{\hbar^2}{2m} \nabla'^2 + V') \psi' \psi \right\}$$

$$= \int d^3r' \underbrace{(\psi \psi^{+\prime} - \psi^{+\prime} \psi)}_{\underset{(6a)}{=} \delta^3(\vec{r} - \vec{r}')} (-\tfrac{\hbar^2}{2m} \nabla'^2 + V') \psi'$$

$$\Rightarrow [\hat{\psi}, \hat{H}]_- = \left(-\frac{\hbar^2}{2m} \nabla^2 + V\right) \psi$$

$\boxed{\text{Summary:}}$ The eq. of motion for the quantum field operator $\hat{\psi}(\vec{r}, t)$ is

$$\boxed{i\hbar \frac{d\hat{\psi}(\vec{r},t)}{dt} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r},t)\right) \hat{\psi}(\vec{r},t)} \quad \underline{(8)}$$

which we may regard as the <u>"second-quantized" Schrödinger eq.</u> for the <u>field operator $\hat{\psi}(\vec{r},t)$.</u> In this approach, the "ordinary Schrödinger eq." for the "class." field $\psi(\vec{r},t)$ is the "first-quantized" version.

The <u>second-quantized one-body Hamiltonian $\hat{H}$</u> can be written in the form

$$\boxed{\hat{H} = \int d^3r \underset{\text{field op.}}{\hat{\psi}^+(\vec{r},t)} \underset{\text{s.p. operator}}{\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r},t)\right)} \underset{\text{field op.}}{\hat{\psi}(\vec{r},t)}} \quad \underline{(9)}$$

which is exactly the same result as the one-body part of the many-particle Hamiltonian in occup. # representation (see ch. 2, p. 27).

$\boxed{\text{\underline{Conclusion}: nonrel. quantum field theory is equivalent to nonrel. many-particle quantum theory!}}$

Wick's theorem and applications

Lit: FW, p. 86–92
Blaizot & Ripka, p. 88–90
Ring & Schuck, Appendix C4

Purpose: Wick's theorem was developed for QFT to evaluate g.s./vacuum expectation values of quantum field operators such as

$$\langle \Phi_0 | \underbrace{T}_{\text{time-ordered product}} \{ \hat{\psi}^+_\lambda (\underbrace{x_1}_{\text{4-d spacetime}}) \hat{\psi}^+_\mu (x_1') \ldots \hat{\psi}_\alpha(x) \underbrace{\hat{\psi}^+_\beta}_{\text{field operator}}(y) \} | \Phi_0 \rangle$$

We will encounter such quantities later in the perturbative approach to many-body QT.

Wick's theorem may also be used for the special case of time-indep. creation/annih. operators:

$$\langle \phi_0^{HF} | \hat{c}^+_\alpha \hat{c}^+_\beta \hat{c}_\delta \hat{c}_\gamma | \phi_0^{HF} \rangle \quad \text{etc.}$$

which appear in the HF theory.

Def. of T-product

The time-ordered product of time-dep. operators is defined by a reordering such that time arguments are increasing from right to left; for example if $t_1 > t_2 > t_3 > t_4$, then:

$$T\Big(A(t_1)\, B(t_3)\, C(t_2)\, D(t_4)\Big) = \delta_P \times A(t_1)\, C(t_2)\, B(t_3)\, D(t_4)$$

The phase factor δ_p is obtained as follows:

for boson operators : $\delta_p = +1$

for fermion operators : $\delta_p = \begin{cases} +1, & \text{for even permutation} \\ -1, & \text{for odd permutation} \end{cases}$

We also define the distributive property:

$$T(A+B) = T(A) + T(B)$$

$\boxed{\text{Def. of } N\text{-product: } N(ABCD\ldots) = \delta_p N(CADB\ldots)}$

"normal-ordered"

The operators are ordered in such a way that all creation operators are to the left of all destruction operators, with the phase factor δ_p as in the T-product. For example, if we have 4 fermion operators

$$N\left(\hat{a}_\nu \hat{a}_\mu \hat{a}_\rho \hat{a}_\sigma^+\right) = -\hat{a}_\sigma^+ \hat{a}_\nu \hat{a}_\mu \hat{a}_\rho$$

3 successive permutations of fermions ($\delta_p = -1$).

and again the distributive property

$$N(A+B) = N(A) + N(B)$$

Def. of contraction

The contraction of 2 operators A and B, denoted here as $\underbrace{A\ B}$, is defined as the difference between the T and N-product:

$$\underbrace{AB} \stackrel{\text{def}}{=} T(AB) - N(AB)$$

Example, useful for HF theory. Suppose we have time-indep.

creation / destr. operators $\hat{a}_\alpha$, $\hat{b}_\alpha$ (like in the HF theory).
In this case one defines

$$\underset{\text{time-indep}}{T}(\hat{a}_\mu \hat{a}_\nu^+) = \underline{\text{given order} = a_\mu a_\nu^+} \quad \text{so that}$$

the contraction becomes

$$\boxed{\underbrace{\hat{a}_\mu \hat{a}_\nu^+}} = T(\hat{a}_\mu \hat{a}_\nu^+) - N(\hat{a}_\mu \hat{a}_\nu^+) \quad \text{1 fermion permutation } (-1)$$

$$= \hat{a}_\mu \hat{a}_\nu^+ \underline{+} N(\hat{a}_\nu^+ \hat{a}_\mu)$$

$$= \hat{a}_\mu \hat{a}_\nu^+ + \hat{a}_\nu^+ \hat{a}_\mu = \boxed{\delta_{\mu\nu}}$$

This simple example illustrates that the contractions are, in most cases of interest, simple c-numbers. We illustrate this with an important example from HF theory. Let's calculate the g.s. expectation value

$$\left.\begin{aligned} \langle \phi_0 | \underbrace{\hat{c}_\alpha^+ \hat{c}_\beta}_{a,b} | \phi_0 \rangle &= \langle \phi_0 | T_{a,b}(\hat{c}_\alpha^+ \hat{c}_\beta) | \phi_0 \rangle \\ &\quad - \langle \phi_0 | N_{a,b}(\hat{c}_\alpha^+ \hat{c}_\beta) | \phi_0 \rangle \end{aligned}\right\} \quad (*)$$

where the notation $\underbrace{\quad}_{a,b}$, $T_{a,b}$ and $N_{a,b}$ mean that the contraction, T-product and N-product are defined with respect to the p/h operators $\hat{a}, \hat{b}$ after the can. transf. $\hat{c}_\alpha \to (\hat{a}_\alpha, \hat{b}_\alpha)$ has been carried out.
Note that the above g.s. exp. value of the N-product always vanishes because $\langle \phi_0 | N_{a,b}(\hat{c}_\alpha^+ \hat{c}_\beta) | \phi_0 \rangle$ has the form

either: $\langle\phi_0|\ldots\underbrace{\hat{a}|\phi_0\rangle}_{=0}$ or $\langle\phi_0|\ldots\underbrace{\hat{b}|\phi_0\rangle}_{=0}$

or: $\underbrace{\langle\phi_0|\hat{a}^+}_{=0}\ldots|\phi_0\rangle$ or $\underbrace{\langle\phi_0|\hat{b}^+}_{=0}\ldots|\phi_0\rangle$

therefore we obtain for the contraction

$$\langle\phi_0|\underbrace{\hat{c}_\alpha^+\hat{c}_\beta}_{a,b}|\phi_0\rangle = \langle\phi_0|\underbrace{T_{a,b}(\hat{c}_\alpha^+\hat{c}_\beta)}_{=\text{given order}}|\phi_0\rangle - 0$$
$$= \langle\phi_0|\hat{c}_\alpha^+\hat{c}_\beta|\phi_0\rangle$$

[ch. 3, p. 8]

According to our calculation using the p-h transf. ~~[illegible]~~ the matrix element on the right is the c-number $\rho_{\beta\alpha} = \theta(\varepsilon_F-\varepsilon_\alpha)\delta_{\alpha\beta}$. So, again the contraction is a c-number, and we have established the important result:

$$\boxed{\underbrace{\hat{c}_\alpha^+\hat{c}_\beta} = \langle\phi_0|\hat{c}_\alpha^+\hat{c}_\beta|\phi_0\rangle = \theta(\varepsilon_F-\varepsilon_\alpha)\delta_{\alpha\beta} \overset{\text{def}}{=} \rho_{\beta\alpha}} \quad (*)$$

Note that the contraction is defined with respect to the p-h operators $\hat{a}_\alpha, \hat{b}_\alpha$ with the property

$$\boxed{\hat{a}_\alpha|\phi_0\rangle = 0 = \hat{b}_\alpha|\phi_0\rangle}$$

Wick's theorem (proof e.g. FW p. 90-92)

$$T(ABCD\ldots) = N(ABCD\ldots) + \sum_{\substack{\text{single}\\ \text{contraction}}} N(AB\underbrace{CD}\ldots)$$

$$+ \sum_{\substack{\text{double}\\ \text{contraction}}} N(ABCD\ldots) + \sum_{\substack{\text{full}\\ \text{contraction}}} N(ABCD\ldots)$$

This is best illustrated with an example for 4 time-indep. fermion operators A, B, C, D:

$$
\left\{
\begin{aligned}
T(ABCD) = {} & N(ABCD) + && \text{no contraction} \\
& + N(\underbracket{AB}CD) + N(\underbracket{ABC}D) + N(\underbracket{ABCD}) && \\
& + N(A\underbracket{BC}D) + N(A\underbracket{BCD}) + N(AB\underbracket{CD}) && \text{one contr.} \\
& + N(\underbracket{AB}\,\underbracket{CD}) + N(ABCD) + N(\underbracket{A\underbracket{BC}D}) && \text{full contr.}
\end{aligned}
\right.
$$

Note that if the contractions are c-numbers, it is useful to rearrange the operators inside the N-products such that the contracted operators are next to each other; in this case we get $\pm$ signs for fermion operators, e.g.

$$N(\underset{\text{c-nbr}}{\underbracket{AB}}CD) = \underbracket{AB}\,N(CD)$$

$$N(\underbracket{ABC}D) = -N(\underbracket{AC}BD) = -\underbracket{AC}\,N(BD)$$

$$N(ABCD) = -N(\underbracket{AC}\,\underbracket{BD}) = -\underbracket{AC}\cdot\underbracket{BD} \quad \text{etc.}$$

Hence, we obtain:

$$
\left.
\begin{aligned}
T(ABCD) = {} & N(ABCD) + \underbracket{AB}\,N(CD) \\
& - \underbracket{AC}\,N(BD) + \underbracket{AD}\,N(BC) + \underbracket{BC}\,N(AD) - \underbracket{BD}\,N(AC) + \underbracket{CD}\,N(A,B) \\
& + \underbracket{AB}\,\underbracket{CD} - \underbracket{AC}\,\underbracket{BD} + \underbracket{BC}\,\underbracket{AD}.
\end{aligned}
\right\}
$$

$\boxed{\text{Important application: g.s. expectation value of 2-body operator}}$

Goal: evaluate $\langle \phi_0 | \underbrace{\hat{c}_\alpha^+ \hat{c}_\beta^+ \hat{c}_\delta \hat{c}_\gamma}_{\text{time-indep.}} | \phi_0 \rangle$ ← non-int. g.s.

Reason: a) this exp. value appears in the theory of the interacting electron gas ($e^- e^-$ int.), see ch. 5.

b) expression appears in calculation of pair correlation function of fermions, see ch. 6.

c) expression appears in Hartree-Fock theory, see ch. 7.

From p. 10: $T(\hat{c}_\alpha^+ \hat{c}_\beta^+ \hat{c}_\delta \hat{c}_\gamma)$ = given order $= \hat{c}_\alpha^+ \hat{c}_\beta^+ \hat{c}_\delta \hat{c}_\gamma$

time-indep.

Therefore:

$$\langle \phi_0 | \hat{c}_\alpha^+ \hat{c}_\beta^+ \hat{c}_\delta \hat{c}_\gamma | \phi_0 \rangle = \langle \phi_0 | T(\hat{c}_\alpha^+ \hat{c}_\beta^+ \hat{c}_\delta \hat{c}_\gamma) | \phi_0 \rangle =$$

Wick's theorem for 4 fermion ops, p. 12 =

$$= \langle \phi_0 | N(\hat{c}_\alpha^+ \hat{c}_\beta^+ \hat{c}_\delta \hat{c}_\gamma) | \phi_0 \rangle + \qquad \text{no contraction}$$

$$\left. \begin{aligned} &\underbrace{\hat{c}_\alpha^+ \hat{c}_\beta^+} \langle \phi_0 | N(\hat{c}_\delta \hat{c}_\gamma) | \phi_0 \rangle + \dots + \\ &\underbrace{\hat{c}_\delta \hat{c}_\gamma} \langle \phi_0 | N(\hat{c}_\alpha^+ \hat{c}_\beta^+) | \phi_0 \rangle \end{aligned} \right\} \text{6 single contractions}$$

$$\left. \begin{aligned} &+ \underbrace{\hat{c}_\alpha^+ \hat{c}_\beta^+} \cdot \underbrace{\hat{c}_\delta \hat{c}_\gamma} - \underbrace{\hat{c}_\alpha^+ \hat{c}_\delta} \cdot \underbrace{\hat{c}_\beta^+ \hat{c}_\gamma} \\ &+ \underbrace{\hat{c}_\beta^+ \hat{c}_\delta} \cdot \underbrace{\hat{c}_\alpha^+ \hat{c}_\gamma} \end{aligned} \right\} \text{3 double contractions}$$

But note that the g.s. expectation values of all normal-ordered products vanish in the non-int. ground state (see top of p. 11), hence:

$$\langle\phi_0|\hat{c}_\alpha^+\hat{c}_\beta^+\hat{c}_\delta\hat{c}_\gamma|\phi_0\rangle = \text{full contractions only} =$$

$$= \underbrace{\hat{c}_\alpha^+\hat{c}_\beta^+}_{\substack{=K^*_{\alpha\beta}=0\\ \text{(see below)}}}\cdot\underbrace{\hat{c}_\delta\hat{c}_\gamma}_{\substack{=K_{\gamma\delta}=0\\ \text{(see below)}}} - \underbrace{\hat{c}_\alpha^+\hat{c}_\delta}_{=\rho_{\delta\alpha}}\cdot\underbrace{\hat{c}_\beta^+\hat{c}_\gamma}_{=\rho_{\gamma\beta}} + \underbrace{\hat{c}_\beta^+\hat{c}_\delta}_{=\rho_{\delta\beta}}\cdot\underbrace{\hat{c}_\alpha^+\hat{c}_\gamma}_{=\rho_{\gamma\alpha}}$$

Summary: g.s. expectation value of 2-body operator

$$\langle\phi_0|\hat{c}_\alpha^+\hat{c}_\beta^+\hat{c}_\delta\hat{c}_\gamma|\phi_0\rangle = \text{Wick's theorem} =$$

$$= -\rho_{\delta\alpha}\cdot\rho_{\gamma\beta} + \rho_{\delta\beta}\cdot\rho_{\gamma\alpha}$$

where (see ch. 3, p. 8; ch. 4, p. 11): $\boxed{\rho_{\beta\alpha} = \Theta(\varepsilon_F - \varepsilon_\alpha)\,\delta_{\alpha\beta}}$

"Pairing tensor" matrix elements $K_{\gamma\delta}$

We define

$$K_{\gamma\delta} \stackrel{\text{def}}{=} \langle\phi_0|\hat{c}_\delta\hat{c}_\gamma|\phi_0\rangle \equiv \underbrace{\hat{c}_\delta\hat{c}_\gamma}$$

Theorem: for non-int. g.s. $|\phi_0\rangle$, the pairing tensor matrix elements vanish, i.e.

$$\boxed{K_{\gamma\delta}\equiv 0}$$ Proof: → homework!

Theorem: $\underbrace{\hat{c}_\alpha^+ \hat{c}_\beta^+} = K^*_{\alpha\beta}$

Proof: $\underbrace{\hat{c}_\alpha^+ \hat{c}_\beta^+} = \langle \phi_0 | \hat{c}_\alpha^+ \hat{c}_\beta^+ | \phi_0 \rangle = \langle (\hat{c}_\alpha^+ \hat{c}_\beta^+)^+ \phi_0 | \phi_0 \rangle =$

$$= \langle \underbrace{\hat{c}_\beta \hat{c}_\alpha \phi_0}_{=a} | \underbrace{\phi_0}_{b} \rangle \underset{\substack{\uparrow \\ \text{use} \\ \langle a|b\rangle = \langle b|a\rangle^*}}{=} \langle \phi_0 | \hat{c}_\beta \hat{c}_\alpha | \phi_0 \rangle^* \overset{\text{def}}{=} K^*_{\alpha\beta}.$$

Conclude: in non-int. g.s., $\underbrace{\hat{c}_\alpha^+ \hat{c}_\beta^+} = K^*_{\alpha\beta} \equiv 0$
(from last theorem).

Remark: The pairing tensor matrix elements vanish in the "simple" non-int. g.s. $|\phi_0\rangle$, but they are non-zero in the BCS-theory (see later, ch. 9 and Fetter/Walecka, §37).