Expectation Values, Wick's Theorem and Normal Ordering

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In this paper we consider expectation values for Hamiltonians bilinear in the fields. These expectation values are closely related to normal ordering, which was used by Wick [1] to determine expectation values for the quantum case. There are various approaches to obtain these results. An alternative approach which allows an algebraic formulation for perturbation theory can be found for example in [2]. The author does not claim, that the material given below is new.

1 Expectation values for bilinear Hamiltonians

In this section a systematic way to evaluate the expectation values of products of fields for Hamiltonians bilinear in the fields is given. This holds both for classical (commuting and anti-commuting) and for quantum fields (bosons and fermions). As a result the expectation value can be expressed as the sum (21 and 46).

1.1 Classical Fields

1.1.1 Real Fields

First we consider a Hamiltonian H bilinear in real fields ϕ

$$H = \frac{1}{2}\sum_{kl} \phi_k M_{kl} \phi_l. \tag{1}$$

The matrix M is assumed to be symmetric. We assume moreover that the real parts of the eigenvalues of M are positive. Then the integral over the partial derivative

$$\int D\phi \, \frac{\partial}{\partial \phi_m}(A(\phi)e^{-H}) = 0 \tag{2}$$

vanishes where $\int D\phi$ stands for the integral over all ϕ_k from $-\infty$ to $+\infty$. It is assumed, that $A(\phi)$ does not increase too fast (a polynomial increase is allowed). Evaluation of the derivative yields

$$\int D\phi \, \frac{\partial A}{\partial \phi_m} e^{-H} = \int D\phi \, \sum_l M_{ml}\phi_l A(\phi) e^{-H}. \tag{3}$$

After division by the partition function $\int D\phi e^{-H}$ we obtain for the expectation values

$$< \frac{\partial A(\phi)}{\partial \phi_m} >= \sum_l M_{ml} < \phi_l A(\phi) > . \tag{4}$$

Multiplication of this equation by M^{-1} yields

$$< \phi_m A(\phi) >= \sum_l (M^{-1})_{ml} < \frac{\partial A(\phi)}{\phi_l} > . \tag{5}$$

In particular for $A = \phi_n$ one obtains

$$< \phi_m \phi_n >= (M^{-1})_{mn} \tag{6}$$

and thus

$$< \phi_m A(\phi) >= \sum_l < \phi_m \phi_l >< \frac{\partial A(\phi)}{\partial \phi_l} >, \tag{7}$$

which is our result.

1.1.2 Complex Fields

Similarly one may introduce a Hamiltonian

$$H = \sum_{kl} \phi_k^\star M_{kl} \phi_l \tag{8}$$

In order to evaluate the partition function or expectation values one has to integrate independently over the real and the imaginary parts of the ϕ_k. Thus

$$D\phi = \prod_k (d\Re\phi_k d\Im\phi_l). \tag{9}$$

The derivatives are defined so that

$$\frac{\partial \phi}{\partial \phi} = 1,\ \frac{\partial \phi}{\partial \phi^\star} = 0,\ \frac{\partial \phi^\star}{\partial \phi} = 0,\ \frac{\partial \phi^\star}{\partial \phi^\star} = 1. \tag{10}$$

This can be achieved with

$$\frac{\partial}{\partial \phi} = \frac{1}{2}(\frac{\partial}{\partial \Re\phi} - i\frac{\partial}{\partial \Im\phi}),\ \frac{\partial}{\partial \phi^\star} = \frac{1}{2}(\frac{\partial}{\partial \Re\phi} + i\frac{\partial}{\partial \Im\phi}). \tag{11}$$

Then the derivation of

$$\begin{aligned} < \phi_m \phi_n^\star > &= (M^{-1})_{mn}, & (12)\\ < \phi_m^\star A > &= \sum_l < \phi_m^\star \phi_l >< \frac{\partial A}{\partial \phi_l} >, & (13)\\ < \phi_m A > &= \sum_l < \phi_m \phi_l^\star >< \frac{\partial A}{\partial \phi_l^\star} > . & (14)\end{aligned}$$

runs parallel to that given for real fields. A more general Hamiltonian is

$$H = \sum_{kl} \phi_k^\star M_{kl} \phi_l + \frac{1}{2}\sum_{kl} \phi_k^\star M'_{kl} \phi_l^\star + \frac{1}{2}\sum_{kl} \phi_k M''_{kl} \phi_l \tag{15}$$

with symmetric M' and M''. Then

$$\begin{aligned} < \phi_m^\star A > &= \sum_l < \phi_m^\star \phi_l >< \frac{\partial A}{\partial \phi_l} > + \sum_l < \phi_m^\star \phi_l^\star >< \frac{\partial A}{\partial \phi_l^\star} >, & (16)\\ < \phi_m A > &= \sum_l < \phi_m \phi_l >< \frac{\partial A}{\partial \phi_l} > + \sum_l < \phi_m \phi_l^\star >< \frac{\partial A}{\partial \phi_l^\star} > . & (17)\end{aligned}$$

Basically $\phi^\star$ and ϕ can be considered to be independent fields.

1.1.3 Grassmannian Fields and Superfields

In classical electrodynamics the electromagnetic field is described by real fields. In quantum electrodynamics the fields are quantized and described by bosonic creation and annihilation operators. Our world consists not only of bosons but also of fermions. The classical counterpart of fermionic fields are Grassmann variables which anticommute. One can also introduce a Hamiltonian H, eq. (1) for anticommuting fields. If the fields ϕ are Grassmannian, then M has to be antisymmetric. We require that M^{-1} exists. Then M has to be of even dimension. Noting that the integral over Grassmannian fields is defined by

$$\int d\phi A = \frac{\partial A}{\partial \phi} \tag{18}$$

it is obvious that eq.(2) holds for Grassmannian fields too, since the second derivative with respect to a Grassmannian variable vanishes, since due to the anticommutativity the square of a Grassmann variable vanishes. Then the derivation of eq. (7) is completely analogous. For $A(\phi)$ one chooses an odd element of the algebra. Odd (even) means a sum of products each of which contains in total an odd (even) number of Grassmann variables. One may also choose both commuting and anticommuting fields (superfields). If ϕ_k is commuting and ϕ_l is anticommuting, then $M_{kl} = -M_{lk}$ should be odd elements of the algebra, so that H is an even element of the algebra.

1.1.4 Remarks

Let us denote a linear combination of fields ϕ and $\phi^\star$ by γ. Then apparently

$$< \gamma A >= \sum_l < \gamma\phi_l >< \frac{\partial A}{\partial \phi_l} > + \sum_l < \gamma\phi_l^\star >< \frac{\partial A}{\partial \phi_l^\star} > \tag{19}$$

holds. Using the identity

$$\sum_l \phi_l \frac{\partial}{\partial \phi_l}\gamma + \sum_l \phi_l^\star \frac{\partial}{\partial \phi_l^\star}\gamma = \gamma. \tag{20}$$

we obtain for a product of fields γ

$$< \gamma_1\gamma_2...\gamma_{2n} >= \sum_{k=2}^{2n} (\pm)^k < \gamma_1\gamma_k >< \prod_{l=2, l\neq k}^{2n} \gamma_l >, \tag{21}$$

which yields recursively a sum of $(2n-1)!!$ products of n factors $< \gamma_k\gamma_l >$. The upper sign holds for commuting fields, the lower for anticommuting ones. In the case of the Hamiltonian (8) the number of terms reduces to $n!$, since no anomalous terms $< \phi\phi >$ and $< \phi^\star\phi^\star >$ appear. This expansion is often referred to as Wick's theorem.

1.2 Quantum Fields

1.2.1 Bosons

We show, that a similar theorem holds for a Hamiltonian H which is bilinear in the creation and annihilation operators $c^\dagger$ and c of bosons in the form

$$\begin{aligned} < c_k^\dagger A > &= -\sum_l < c_k^\dagger c_l >< [c_l^\dagger, A] > + \sum_l < c_k^\dagger c_l^\dagger >< [c_l, A] >, & (22)\\ < c_k A > &= -\sum_l < c_k c_l >< [c_l^\dagger, A] > + \sum_l < c_k c_l^\dagger >< [c_l, A] > . & (23) \end{aligned}$$

We start with

$$0 = \mathrm{tr}([c_k^\dagger, Ae^{-\beta H}]) = \mathrm{tr}([c_k^\dagger, A]e^{-\beta H}) + \mathrm{tr}(A[c_k^\dagger, e^{-\beta H}]) \tag{24}$$

and a similar equation in which $c_k^\dagger$ is replaced by c_k.

In a next step we have to evaluate the commutator $[c_k^\dagger, e^{-\beta H}]$. We introduce the column vector $\begin{pmatrix} c^\dagger \\ c \end{pmatrix}$. Since the commutator with H is linear in the creation and annihilation operators, we may write

$$[\begin{pmatrix} c^\dagger \\ c \end{pmatrix}, H] = -M \begin{pmatrix} c^\dagger \\ c \end{pmatrix} \tag{25}$$

with a coefficient matrix M, which within a Lie algebra is denoted by ad$H$. From this we obtain

$$\begin{pmatrix} c^\dagger \\ c \end{pmatrix}(1-\alpha H) = (1-\alpha H)(1+\alpha M)\begin{pmatrix} c^\dagger \\ c \end{pmatrix} + O(\alpha^2). \tag{26}$$

From $e^{-\beta H} = \lim_{n\to\infty}(1-\frac{\beta H}{n})^n$ one obtains

$$\begin{pmatrix} c^\dagger \\ c \end{pmatrix} e^{-\beta H} = e^{-\beta H} e^{\beta M} \begin{pmatrix} c^\dagger \\ c \end{pmatrix} \tag{27}$$

and therefore

$$\begin{aligned} \mathrm{tr}(A[\begin{pmatrix} c^\dagger \\ c \end{pmatrix}, e^{-\beta H}]) &= (e^{\beta M}-1)\mathrm{tr}(\begin{pmatrix} c^\dagger \\ c \end{pmatrix} A e^{-\beta H}), & (28) \\ <[\begin{pmatrix} c^\dagger \\ c \end{pmatrix}, A]> &= (1-e^{\beta M}) < \begin{pmatrix} c^\dagger \\ c \end{pmatrix} A > & (29) \end{aligned}$$

or

$$< \begin{pmatrix} c^\dagger \\ c \end{pmatrix} A >= (1-e^{\beta M})^{-1} <[\begin{pmatrix} c^\dagger \\ c \end{pmatrix}, A]> . \tag{30}$$

I introduce now in place of A the row vector $\begin{pmatrix} -c & c^\dagger \end{pmatrix}$ where transposition is not explicitly indicated. Then

$$<[\begin{pmatrix} c^\dagger \\ c \end{pmatrix}, A]>=< \begin{pmatrix} [c^\dagger, -c] & [c^\dagger, c^\dagger] \\ [c, -c] & [c, c^\dagger] \end{pmatrix} > \tag{31}$$

is the unit matrix and thus

$$< \begin{pmatrix} c^\dagger \\ c \end{pmatrix} \begin{pmatrix} -c & c^\dagger \end{pmatrix} >= (1-e^{\beta M})^{-1} \tag{32}$$

which yields for bosons

$$< \begin{pmatrix} c^\dagger \\ c \end{pmatrix} A >=< \begin{pmatrix} c^\dagger \\ c \end{pmatrix} \begin{pmatrix} -c & c^\dagger \end{pmatrix} >< [\begin{pmatrix} c^\dagger \\ c \end{pmatrix}, A]> . \tag{33}$$

If written in components one has the form as given above in eqs.(22) and (23).

1.2.2 Fermions

For fermions the derivation has to be modified. Then one obtains

$$\begin{aligned} < c_k^\dagger A > &= \sum_l < c_k^\dagger c_l >< \{c_l^\dagger, A\} > + \sum_l < c_k^\dagger c_l^\dagger >< \{c_l, A\} >, & (34) \\ < c_k A > &= \sum_l < c_k c_l >< \{c_l^\dagger, A\} > + \sum_l < c_k c_l^\dagger >< \{c_l, A\} > . & (35) \end{aligned}$$

Since the only nonvanishing contributions come from products of an even number of creation and annihilation operators, A has to contain products of an odd number of such operators. Therefore I introduce the anticommutators $\{c^\dagger, A\}$ and $\{c, A\}$ and have

$$0 = \mathrm{tr}([c_k^\dagger, A e^{-\beta H}]) = \mathrm{tr}(\{c_k^\dagger, A\} e^{-\beta H}) - \mathrm{tr}(A\{c_k^\dagger, e^{-\beta H}\}). \tag{36}$$

Analogously to the bosons eqs.(25,26,27) hold for fermions. Therefore one obtains

$$\mathrm{tr}(A\{\begin{pmatrix} c^\dagger \\ c \end{pmatrix}, e^{-\beta H}\}) = (e^{\beta M}+1) < \begin{pmatrix} c^\dagger \\ c \end{pmatrix} A > \tag{37}$$

or

$$< \begin{pmatrix} c^\dagger \\ c \end{pmatrix} A >= (1+e^{\beta M})^{-1} < \{\begin{pmatrix} c^\dagger \\ c \end{pmatrix}, A\} > . \tag{38}$$

With $A = \begin{pmatrix} c & c^\dagger \end{pmatrix}$ this yields

$$< \{\begin{pmatrix} c^\dagger \\ c \end{pmatrix}, A\} >=< \begin{pmatrix} \{c^\dagger, c\} & \{c^\dagger, c^\dagger\} \\ \{c, c\} & \{c, c^\dagger\} \end{pmatrix} > \tag{39}$$

with the right hand side being the unit matrix, so that

$$< \begin{pmatrix} c^\dagger \\ c \end{pmatrix} \begin{pmatrix} c & c^\dagger \end{pmatrix} >= (1+e^{\beta M})^{-1}. \tag{40}$$

Thus we obtain

$$< \begin{pmatrix} c^\dagger \\ c \end{pmatrix} A >=< \begin{pmatrix} c^\dagger \\ c \end{pmatrix} \begin{pmatrix} c & c^\dagger \end{pmatrix} >< \{\begin{pmatrix} c^\dagger \\ c \end{pmatrix}, A\} >, \tag{41}$$

which are the equations (34) and (35) for fermions.

1.2.3 Remarks

(i) Especially for a diagonal Hamiltonian $H = \sum_k \epsilon_k c_k^\dagger c_k$ M becomes diagonal with $M = \begin{pmatrix} \epsilon & 0 \\ 0 & -\epsilon \end{pmatrix}$. From these one obtains the well-known distributions of bosons and fermions.

(ii) Obviously a linear combination γ of operators $c^\dagger$ and c obeys

$$< \gamma A >= -\sum_l < \gamma c_l >< [c_l^\dagger, A] > + \sum_l < \gamma c_l^\dagger >< [c_l, A] > \tag{42}$$

for bosons and

$$< \gamma A >= \sum_l < \gamma c_l >< \{c_l^\dagger, A\} > + \sum_l < \gamma c_l^\dagger >< \{c_l, A\} > \tag{43}$$

for fermions. Moreover a linear combination γ' of operators $c^\dagger$ and c reproduces under the operation

$$-\sum_l c_l[c_l^\dagger, \gamma'] + \sum_l c_l^\dagger [c_l, \gamma'] = \gamma' \tag{44}$$

for bosons and

$$\sum_l c_l\{c_l^\dagger, \gamma'\} + \sum_l c_l^\dagger \{c_l, \gamma'\} = \gamma' \tag{45}$$

for fermions. Thus for a product of such operators γ_l one has

$$< \gamma_1\gamma_2 ... \gamma_{2n} >= \sum_{k=2}^{2n} (\pm)^k < \gamma_1\gamma_k >< \prod_{l=2, l\neq k}^{2n} \gamma_l >, \tag{46}$$

which yields recursively a sum of $(2n-1)!!$ products of n factors $< \gamma_k\gamma_l >$. The upper sign holds for bosons, the lower for fermions. In the original version of Wick the creation and annihilation operators are often rotated by H, $a_k(t) = e^{iHt}a_k e^{-iHt}$. These time-dependent operators are still linear in the original ones due to eq. (27).

(iii) Comparing the theorem for classical fields eqs. (7, 13-14,16-17) with that of quantum fields eqs. (22-23, 34-35) we observe that in the classical case we have on the right hand side the derivative of A with respect to a field whereas in the quantum case we have the (anti-)commutator of a creation or annihilation operator with A. We note, that the (anti-)commutator has basically the same effect like a derivative since the (anti-)commutator with a creation operator removes an annihilation operator and vice versa from a product of operators.

2 Wick's theorems and Normal Ordering

2.1 Bosons

2.1.1 Definition of normal ordering

In this section Wick's theorems [1] and the normal ordering of Bose fields are introduced. In the following I denote by a_k any linear combination of Bose creation and annihilation operators. I introduce a matrix G, which normally describes the correlations of the operators a for a Hamiltonian H bilinear in the creation and annihilation operators (free theory)

$$< a_k a_l >= G_{kl} \tag{47}$$

These matrix-elements are called contractions. What we really need for the definition of normal ordering is only, that the commutator of the operators obeys

$$[a_k, a_l] = G_{kl} - G_{lk} \tag{48}$$

The following is also valid for classical commutating fields for which of course $G_{kl} = G_{lk}$.

Normal ordering of an operator A denoted by $: A :$ is now defined by

$$\begin{aligned} :1: &= 1, && (49)\\ :\alpha A(a) + \beta B(a): &= \alpha : A(a) : + \beta : B(a) :, && (50)\\ a_k : A(a) : &= : a_k A(a) : + \sum_l G_{kl} : \frac{\partial A(a)}{\partial a_l} : && (51) \end{aligned}$$

where α and β are c-numbers. The second of these three equations defines normal ordering as a linear procedure. (rule A of Wick). The third one is a recurrence relation (mentioned by Wick after rule C", who however introduces multiplication of a_k from the right), and the first one sets the initial step.

2.1.2 Product of two normal ordered operators

We may now iterate the third equation

$$\begin{aligned} a_k : A(a) : &= : (a_k + \sum_{kl} G_{kl} \frac{\partial}{\partial a_l}) A(a) : && (52)\\ a_{k_1} a_{k_2} : A(a) : &= : (a_{k_1} + \sum_{l_1} G_{k_1 l_1} \frac{\partial}{\partial a_{l_1}})(a_{k_2} + \sum_{l_2} G_{k_2 l_2} \frac{\partial}{\partial a_{l_2}}) A(a) : && (53) \end{aligned}$$

from which we conclude

$$a_{k_1} a_{k_2} ... a_{k_m} =: (a_{k_1} + \sum_{l_1} G_{k_1 l_1} \frac{\partial}{\partial a_{l_1}})(a_{k_2} + \sum_{l_2} G_{k_2 l_2} \frac{\partial}{\partial a_{l_2}}) ... a_{k_m} : \tag{54}$$

which can also be written as

$$a_{k_1} a_{k_2} ... a_{k_m} =: \exp(\sum G_{kl} \frac{\partial^2}{\partial a_k^{left} \partial a_l^{right}}) a_{k_1} a_{k_2} ... a_{k_m} : . \tag{55}$$

This is Wicks first theorem. The superscripts ^{left} and ^{right} indicate that we always pick a pair of factors a and perform the derivative $\partial/\partial a_k$ on the left factor and the derivative $\partial/\partial a_l$ on the right factor, so that the factor G_{kl} depends on the sequence of the operators. The exponential appears in the equation for the following reason. If we perform the operation $G\partial^2/\partial a \partial a$ on m pairs of factors a, then there are due to the permutation symmetry $m!$ contributions. Therefore in order to obtain the contribution with factor one we have to divide the m-th power of $G\partial^2/\partial a \partial a$ by $m!$, which yields the exponential.

Similarly one obtains

$$: a_{k_1}a_{k_2}...a_{k_m} := \exp(-\sum G_{kl}\frac{\partial^2}{\partial a_k^{left}\partial a_l^{right}})a_{k_1}a_{k_2}...a_{k_m}. \tag{56}$$

In order to obtain the product of two normal ordered operators one can combine

$$: A(a) :: B(a) := \exp(\sum G_{kl}(-\frac{\partial^2}{\partial a_k^{left}\partial a_l^{right}} - \frac{\partial^2}{\partial b_k^{left}\partial b_l^{right}}))A(a)B(b)|_{b=a} \tag{57}$$

and

$$A(a)B(b) =: \exp(\sum G_{kl}(\frac{\partial^2}{\partial a_k^{left}\partial a_l^{right}} + \frac{\partial^2}{\partial b_k^{left}\partial b_l^{right}} + \frac{\partial^2}{\partial a_k\partial b_l}))A(a)B(b) : \tag{58}$$

which yields the **formula for the product of two normal ordered operators**

$$: A(a) :: B(a) :=: \exp(\sum G_{kl}\frac{\partial^2}{\partial a_k\partial b_l})A(a)B(b) : |_{b=a} \tag{59}$$

This is Wick's second theorem.

2.1.3 Commutative Law under Normal Ordering

Now we show, that under normal ordering the commutative law holds. For this purpose we write

$$: a_{k_1}a_{k_2}...a_{k_m} := (a_{k_1} - \sum_{l_1} G_{k_1l_1}\frac{\partial}{\partial a_{l_1}})(a_{k_2} - \sum_{l_2} G_{k_2l_2}\frac{\partial}{\partial a_{l_2}})...a_{k_m} \tag{60}$$

Let us now exchange the factors a_{k_n} and $a_{k_{n+1}}$ on the left hand side of this equation. Then on the right hand side we have to take the commutator

$$\begin{aligned}&[(a_{k_n} - \sum_{l_n} G_{k_nl_n}\frac{\partial}{\partial a_{l_n}}), (a_{k_{n+1}} - \sum_{l_{n+1}} G_{k_{n+1}l_{n+1}}\frac{\partial}{\partial a_{l_{n+1}}})]\\ &= [a_{k_n}, a_{k_{n+1}}] - G_{k_n,k_{n+1}} + G_{k_{n+1}k_n} = 0.\end{aligned} \tag{61}$$

The normal ordered product is invariant under exchange of the two operators a_{k_n} and $a_{k_{n+1}}$ due to eq. (48)

$$: a_{k_1}a_{k_2}...a_{k_n}a_{k_{n+1}}...a_{k_m} :=: a_{k_1}a_{k_2}...a_{k_{n+1}}a_{k_n}...a_{k_m} : \tag{62}$$

Application of this law several times yields generally

$$: ABCD :=: ACBD : . \tag{63}$$

This is rule C of Wick.

2.1.4 Expectation Values

Finally we consider expectation values of normal ordered products with respect to H. I begin with

$$<: a_kA(a) :>=< a_k : A(a) :> - \sum_l G_{kl} <: \frac{\partial A(a)}{\partial a_l} :> \tag{64}$$

The first term on the right hand side of this equation can be written according to eq.(42) and the following remark

$$< a_k : A(a) :>= \sum_l < a_ka_l ><: \frac{\partial A(a)}{\partial a_l} :>, \tag{65}$$

so that both terms cancel,

$$<: a_kA(a) :>= 0 \tag{66}$$

Since all contributions to an operator but a constant can be written as sums of such expressions we obtain

$$<: A(a) :>= A(a = 0). \tag{67}$$

Now suppose P and Q are homogeneous polynomials of order n and m in the fields, resp. Then the product $: P :: Q :$ contains in the normal ordered form terms of order $n+m$, $n+m-2$, ... $|n-m|$ in the fields. Thus $<: P :: Q :>$ vanishes unless $n = m$.

2.2 Other Fields

2.2.1 Classical Fields

The same ideas can be applied for classical fields.

In particular for a real field ϕ we find that apart from an overall factor $: \phi^n :$ is the Hermitean polynomial of order n in ϕ since it is orthogonal with respect to a Gaussian weight function to all $: \phi^m :$ with $m < n$.

For classical fields there is no necessity to distinguish between the superscripts ^{left} and ^{right} in eqs. (55-56). Instead one introduces one half of the unrestricted sum

$$\sum_{kl} G_{kl} \frac{\partial^2}{\partial a_k^{left} \partial a_l^{right}} \to \frac{1}{2} \sum_{kl} G_{kl} \frac{\partial^2}{\partial a_k \partial a_l}. \tag{68}$$

This type of normal ordering is typically e.g. for the eigenoperators in a ϕ^4 theory in first order in $4-d$ in an expansion around d=4 dimensions ([3], eqs. (3.176, 3.177)).

2.2.2 Fermions

For fermions one can basically use the same reasoning. It has only to be considered, that fermions anticommute. Therefore eq. (48) has to be replaced by

$$\{a_k, a_l\} = G_{kl} + G_{lk}. \tag{69}$$

For classical anticommuting fields one has $G_{kl} = -G_{lk}$. It has to be observed that $\frac{\partial}{\partial a_l} a_k = \delta_{kl} - a_k \frac{\partial}{\partial a_l}$ and that in the second derivatives in the exponentials the derivative with respect to a^{left} has to be performed before a^{right}. Thus Wick's theorem eq.(59) has to be written

$$: A(a) :: B(a) :=: \exp(\sum G_{kl} \frac{\partial^2}{\partial b_l \partial a_k}) A(a) B(b) : |_{b=a}. \tag{70}$$

The commutative law under normal ordering eq.(63) reads now

$$: ABCD := \pm : ACBD : \tag{71}$$

where the minus sign applies if B and C are both odd elements of the algebra and the plus sign if B or C is an even element.

2.2.3 Hartree-Fock Approximation

The Hamiltonian of a system of fermions

$$H = \sum_{ks} \epsilon_k c_{ks}^\dagger c_{ks} + \frac{1}{2} \sum_{kk'qss'} V(k,k',q) c_{ks}^\dagger c_{k's'}^\dagger c_{k'+qs'} c_{k-qs} \tag{72}$$

can be rewritten in normal-ordered form as

$$\begin{aligned} H &= E_0 + H_1 + H_2, \qquad (73) \\ E_0 &= \sum_{ks} \epsilon_k < c_{ks}^\dagger c_{ks} > + \frac{1}{2} \sum_{kk'qss'} V(k,k',q) (< c_{ks}^\dagger c_{k-qs} >< c_{k's'}^\dagger c_{k'+qs'} > \end{aligned}$$

$$
\begin{aligned}
& - < c^\dagger_{ks} c_{k'+qs'} >< c^\dagger_{k's'} c_{k-qs} > + < c^\dagger_{ks} c^\dagger_{k's'} >< c_{k'+qs'} c_{k-qs} >), && (74) \\
H_1 &= \sum_{ks} \epsilon_k : c^\dagger_{ks} c_{ks} : + \frac{1}{2} \sum_{kk'qss'} V(k,k',q) \\
& (< c^\dagger_{ks} c_{k-qs} >: c^\dagger_{k's'} c_{k'+qs'} : + < c^\dagger_{k's'} c_{k'+qs'} >: c^\dagger_{ks} c_{k-qs} : \\
& - < c^\dagger_{ks} c_{k'+qs'} >: c^\dagger_{k's'} c_{k-qs} : - < c^\dagger_{k's'} c_{k-qs} >: c^\dagger_{ks} c_{k'+qs'} : \\
& + < c^\dagger_{ks} c^\dagger_{k's'} >: c_{k'+qs'} c_{k-qs} : + < c_{k'+qs'} c_{k-qs} >: c^\dagger_{ks} c^\dagger_{k's'} :), && (75) \\
H_2 &= \frac{1}{2} \sum_{kk'qss'} V(k,k',q) : c^\dagger_{ks} c^\dagger_{k's'} c_{k'+qs'} c_{k-qs} : . && (76)
\end{aligned}
$$

Within the Hartee-Fock scheme the last term H_2 is neglected. The expectation values $< ... >$ are determined as a function of the one-particle Hamiltonian H_1 and the temperature in a self-consistent way. One has to choose the solution with the lowest free energy (including E_0). The second term in E_0 and the second and third term of H_1 are the Hartree- (direct) contributions, the third term in E_0 and the fourth and fifth term in H_1 are the Fock- (exchange) contributions. The fourth term in E_0 and the sixth and seventh term in H_1 are the Bogoliubov- (anomalous) contributions, which appear in the superconducting state.

References

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