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Nonunitary Bogoliubov Transformations and Extension of Wick's Theorem.

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Summary. — Linear transformations are considered, which preserve the (anti-) commutation rules, but not the Hermiticity relation, for (fermion) boson creation and annihilation operators; these transformations lead to Fock space representations on biorthogonal bases of the operator algebra. As an application, an extension of Wick's theorem to matrix elements of an arbitrary operator between two different quasi-particle vacuums is derived. This theorem is useful for calculations which go beyond the variational Hartree-Fock-Bogoliubov methods (H.F.B. with projection, generator co-ordinate method, etc.). A canonical decomposition for Bogoliubov transformations is established, which proves useful, for instance in the calculation of the overlap of two different quasi-particle vacuums.

1. – Introduction and summary.

In the simplest variational approaches of the many-body theory, quasi-particle vacuum states are taken as trial wave functions: quasi-particle operators a_i, $a_i^\dagger$ $(i=1, 2, \ldots, N)$ are first constructed, as canonical linear combinations of the original creation and annihilation operators; the trial wave function is then the corresponding vacuum $|0\rangle_a$. For instance in the Hartree-Fock theory, $|0\rangle_a$ is a Slater determinant; in the Bogoliubov-Valatin (1) theory of superconductivity, $|0\rangle_a$ is a B.C.S. state (2); in the case of bosons, the linear canonical

(1) N. N. Bogoliubov: *Žurn. Èksp. Teor. Fiz.*, **34**, 58 (1958); *Nuovo Cimento*, **7**, 795 (1958); J. G. Valatin: *Nuovo Cimento*, **7**, 843 (1958).
(2) J. Bardeen, L. N. Cooper and J. R. Schrieffer: *Phys. Rev.*, **108**, 1175 (1957).

transformation building a_i and $a_i^\dagger$ is inhomogeneous, so as to describe either Bose condensation (3) or coherent states (4).

Such trial functions do not have in general the same invariance properties as the Hamiltonian. In order to restore the broken invariance, one often projects the state $|0\rangle_a$ on the subspace characterized by the correct quantum numbers (5). The resulting projected state $|\psi\rangle$ is a superposition of various states of the type $|0\rangle_a$. For instance, in the theory of deformed nuclei, the H.F. wave function $|0\rangle_a$ mixes various angular momenta; its projection on a given J is realized by superposing all the $|0\rangle_a$ deduced from one another by rotation (6); similarly the projection of a B.C.S. state (or a boson state) on a subspace with given particle number (2) involves the set of $|0\rangle_a$ deduced from one another by the gauge transformation $a_i \Rightarrow a_i e^{i\varphi}$. In the calculation of $\langle\psi|H|\psi\rangle$, one has then to evaluate quantities of the form ${}_a\langle 0|A|0\rangle_b$, where A is some product of annihilation and creation operators.

More generally, it is necessary to evaluate matrix elements ${}_a\langle 0|A|0\rangle_b$ each time the trial function is a superposition of quasi-particle vacuums. This is the case in the generating co-ordinate method (7), and also for instance in the variational treatment of Anderson's model for localized moments (8).

In the following (Sect. **4**), a generalized Wick's theorem is proved, which simplifies the calculation of such matrix elements. Namely, it will be shown that

$$\langle A\rangle_{ab} \equiv \frac{{}_a\langle 0|A|0\rangle_b}{{}_a\langle 0|0\rangle_b} \tag{1}$$

is expressed, exactly in the same way as for the ordinary Wick's theorem (9), for which $|0\rangle_b = |0\rangle_a$, as the sum of all possible completely contracted products. The nonvanishing contractions are here

$$\langle a_i\rangle_{ab} \tag{2a}$$

(for bosons only), and

$$\overline{a_i a_j} \equiv \langle a_i a_j\rangle_{ab} - \langle a_i\rangle_{ab}\langle a_j\rangle_{ab}\,, \qquad \overline{a_i a_j^\dagger} = \delta_{ij}\,. \tag{2b}$$

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(3) N. N. Bogoliubov: *Žurn. Ėksp. Teor. Fiz.*, **11**, 23 (1947).

(4) R. J. Glauber: *Phys. Rev.*, **131**, 2766 (1963).

(5) P. O. Löwdin: *Phys. Rev.*, **97**, 1509 (1955); R. E. Peierls and J. Yoccoz: *Proc. Phys. Soc.*, A **70**, 381 (1957).

(6) J. Yoccoz: *Proc. Phys. Soc.*, A **70**, 388 (1957).

(7) D. L. Hill and J. A. Wheeler: *Phys. Rev.*, **89**, 1102 (1953); R. E. Peirls and D. J. Thouless: *Nucl. Phys.*, **38**, 154 (1962).

(8) P. W. Anderson; *Phys. Rev.*, **164**, 352 (1968).

(9) G. C. Wick: *Phys. Rev.*, **80**, 268 (1950).

The explicit values of these contractions (eqs. (56-63)), and the overlap ${}_a\langle 0|0\rangle_b$ (eqs. (66, 67)) are also given below in terms of the coefficients of the Bogoliubov transformation $\{a_i, a_i^\dagger\} \Rightarrow \{b_i, b_i^\dagger\}$.

This extension of Wick's theorem to $\langle A\rangle_{ab}$ had already been noticed by Löwdin ([10]) in the special case when $|0\rangle_a$ and $|0\rangle_b$ were Slater determinants, and applied in nuclear physics to describe rotational bands (or R.P.A. vibrations) ([11]). Löwdin's derivation however, based on Sylvester's identity for determinants ([12]), failed for B.C.S. states, and for bosons. Thus, his result could not be applied, for instance, to the calculation of pairing vibrations in nuclei ([13]), since $|0\rangle_a$ and $|0\rangle_b$ are then B.C.S. states. It would be possible to extend his method to that last case, by expressing $|0\rangle_b$ as $\prod_i b_i|0\rangle_a$ (within a normalization factor), and by making use of the extension to Pfaffians ([14]) of Sylvester's identity. In fact, a simpler and quite general method is used in the following.

The main tool will be (Sect. **2**) the introduction of linear transformations $\{a_i, a_i^\dagger\} \Rightarrow \{d_i, \bar{d}_i\}$ which preserve the canonical (anti-) commutation relations, but not necessarily the Hermiticity relation ($\bar{d}_i \neq d_i^\dagger$), thus generalizing the Bogoliubov transformations ([3,15]). To such a transformation on the operator algebra, is associated a simple, but *nonunitary* transformation on the states $|n_1 n_2 \ldots\rangle_a$ of the Fock basis associated to the operators a_i. It yields two biorthogonal bases $|n_1 n_2 \ldots\rangle_d$ and ${}_d\langle\overline{n_1 n_2 \ldots}|$ associated to the operators d_i; in particular, the right and left vacuums $|0\rangle_d$ and $|\bar{0}\rangle_d$ are *not the same state*. We shall take advantage of this freedom (in Sect. **4**) to construct a set of d_i such that $|0\rangle_b$ and ${}_a\langle 0|$ are respectively proportional to $|0\rangle_d$ and ${}_d\langle\bar{0}|$. It will then follow that $\langle A\rangle_{ab} = {}_d\langle\bar{0}|A|0\rangle_d$. For any operator D, product of any number of d_i and $\bar{d}_i$, the extension of Wick's theorem to ${}_d\langle\bar{0}|D|0\rangle_d$ is obvious, since the usual derivation only relies upon the commutation relations of the creation and annihilation operators, and not on their Hermiticity relation. The original creation and annihilation operators being linearly related to the $\{d_i, \bar{d}_i\}$, the extension of Wick's theorem to $\langle A\rangle_{ab}$ follows.

In Sect. **3**, we show that a linear transformation $\mathscr{T}$ on fermion or boson operators (which preserves the commutation relations) is in general equal to

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([10]) P. O. Löwdin: *Phys. Rev.*, **97**, 1474 (1955).

([11]) B. Jancovici and D. H. Schiff: *Nucl. Phys.*, **58**, 678 (1964); H. Rouhaninejad and J. Yoccoz: *Nucl. Phys.*, **78**, 353 (1965); G. Ripka: *Lectures in Theoretical Physics*, vol. **8** C (Boulder, Colo., 1966).

([12]) F. R. Gantmacher: *Matrix Theory* (New York, 1959).

([13]) G. Ripka and R. Padjen: *Nucl. Phys.*, A **132**, 489 (1969).

([14]) E. R. Caianiello: *Nuovo Cimento*, **14**, 177 (1959).

([15]) N. N. Bogoliubov: *Doklady*, **119**, 244 (1958); N. N. Bogoliubov and V. G. Soloviev: *Doklady*, **124**, 1011 (1959); J. G. Valatin: *Phys. Rev.*, **122**, 1012 (1961); F. A. Berezin: *The Method of Second Quantization* (New York, 1966).

a product $\mathscr{T}^{(1)}\mathscr{T}^{(3)}\mathscr{T}^{(2)}$ of simpler transformations (eqs. (37, 42)); $\mathscr{T}^{(1)}$ and $\mathscr{T}^{(2)}$ leave respectively the creation and annihilation operators invariant, and $\mathscr{T}^{(3)}$ affects neither right nor left vacuums. This decomposition differs from those given in refs. [16,17]: in particular, here, even if $\mathscr{T}$ is a usual (unitary) Bogoliubov transformation, the factors $\mathscr{T}^{(1)}$ and $\mathscr{T}^{(2)}$ are nonunitary.

The contents of Sect. **3** is not necessary to the derivation of the extended Wick's theorem (Sect. **4**). It is nevertheless useful for evaluating matrix elements of $\mathscr{T}$ in Fock space, since the principle of the decomposition $\mathscr{T}=\mathscr{T}^{(1)}\mathscr{T}^{(3)}\mathscr{T}^{(2)}$ is to push the creation (annihilation) operators to the left (right). For instance, in Sect. **5**, the explicit value of the overlap ${}_a\langle 0|0\rangle_b$ results immediatately from the application of this decomposition to the Bogoliubov transformation which relates $|0\rangle_a$ to $|0\rangle_b$.

2. – Nonunitary canonical transformations.

Biorthogonal bases. Given an orthogonal basis $|m\rangle_0$ in a Hilbert space, any other (not necessarily orthogonal) basis $|m\rangle_1$ is expressed on the initial basis as

$$|m\rangle_1 = \mathscr{T}|m\rangle_0\,, \tag{3}$$

where $\mathscr{T}$ is a nonsingular operator. The associated basis ${}_1\langle\overline{m}|$, defined by the biorthogonality condition

$${}_1\langle\overline{m}|p\rangle_1 = \delta_{mp}\,, \tag{4}$$

is then given by

$${}_1\langle\overline{m}| = {}_0\langle m|\mathscr{T}^{-1} = {}_1\langle m|(\mathscr{T}\mathscr{T}^\dagger)^{-1}\,. \tag{5}$$

The biorthogonal sets $|m\rangle_1$ and ${}_1\langle\overline{m}|$ also satisfy the closure relation

$$\sum_m |m\rangle_1\,{}_1\langle\overline{m}| = \mathbf{1}\,. \tag{6}$$

Biorthogonal Fock bases. Taking now for the initial basis the Fock basis $|n_1 n_2 \ldots\rangle_a$ associated to the creation and annihilation operators $\{a_i, a_i^\dagger\}$, we perform as in (3) and (5) a nonunitary transformation $\mathscr{T}$, which builds a pair

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([16]) L. K. HUA: *Amer. Journ. Math.*, **66**, 470 (1944); *Harmonic analysis of functions of several complex variables in the classical domains* (published by *Am. Math. Soc.*, 1963). C. BLOCH and A. MESSIAH: *Nucl. Phys.*, **39**, 95 (1962); B. ZUMINO: *Journ. Math. Phys.*, **3**, 1055 (1962); C. BLOCH: *Lectures on the Many-Body Nuclear Problem* (Bombay, 1964).

([17]) R. BALIAN, C. DE DOMINICIS and C. ITZYKSON: *Nucl. Phys.*, **67**, 609 (1965).

of « biorthogonal Fock bases »

$$(3') \qquad |n_1 n_2 \ldots\rangle_c = \mathscr{T}|n_1 n_2 \ldots\rangle_a ,$$

$$(5') \qquad {}_c\langle\overline{n_1 n_2 \ldots}| = {}_a\langle n_1 n_2 \ldots|\mathscr{T}^{-1} .$$

The transformed operators

$$(7a) \qquad c_i \equiv \mathscr{T} a_i \mathscr{T}^{-1} ,$$

$$(7b) \qquad \bar{c}_i \equiv \mathscr{T} a_i^\dagger \mathscr{T}^{-1}$$

satisfy the same canonical (anti-) commutation relations as the a's. The operator $\bar{c}_i$ is no longer the Hermitian conjugate of c_i: $c_i^\dagger \neq \bar{c}_i$. However, the representation of the operator algebra is not modified, since (from eqs. (3'), (5'), (7))

$$(8) \qquad {}_c\langle\overline{n_1' n_2' \ldots}| \begin{pmatrix} c_i \\ \bar{c}_i \end{pmatrix} |n_1 n_2 \ldots\rangle_c = {}_a\langle n_1' n_2' \ldots| \begin{pmatrix} a_i \\ a_i^\dagger \end{pmatrix} |n_1 n_2 \ldots\rangle_a .$$

In particular, the right and left vacuums $|0\rangle_c$ and ${}_c\langle\bar{0}|$ satisfy

$$(9a) \qquad c_i|0\rangle_c = 0 , \qquad {}_c\langle\bar{0}|\bar{c}_i = 0 ,$$

$$(9b) \qquad {}_c\langle\bar{0}|0\rangle_c = 1 ,$$

and the non-Hermitian number operators $\bar{c}_i c_i$ admit (3') and (5') as right and left eigenfunctions.

Generalized Bogoliubov transformations. We restrict now our attention to the transformations $\mathscr{T}$ such that the correspondence (7) is linear (homogeneous for fermions, inhomogeneous for bosons). The infinitesimal generators of this group of $\mathscr{T}$'s are quadratic (and, for bosons, linear) forms of the creation and annihilation operators $\{a_i, a_i^\dagger\}$ (or of $\{c_i, \bar{c}_i\}$). We therefore consider the transformations $\mathscr{T}$ which are exponentials of quadratic (plus, for bosons, linear) forms of these operators. They differ from the usual Bogoliubov transformations [3,15] by their nonunitarity.

As usual, it will be convenient to write each set of operators $\{c_i\}$ and $\{\bar{c}_i\}$ as N-dimensional vectors $\boldsymbol{c}$ and $\bar{\boldsymbol{c}}$, and the whole set as a $2N$-dimensional vector

$$(10) \qquad \boldsymbol{\gamma} \equiv \{\boldsymbol{c}, \bar{\boldsymbol{c}}\} \equiv \{c_1 c_2 \ldots c_N \bar{c}_1 \bar{c}_2 \ldots \bar{c}_N\} .$$

The commutation relations are summarized for fermions by

$$(11) \qquad [\gamma_i, \gamma_j]_+ = \sigma_{ij} ,$$

where σ is the $2N \times 2N$ matrix

$$\sigma \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{12}$$

and for bosons by

$$[\gamma_i, \gamma_j] = \tau_{ij}, \tag{13}$$

with

$$\tau \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{14}$$

Fermion case. The transformation $\mathscr{T}$ may then be written, for fermions, as

$$\mathscr{T} = \exp[\tfrac{1}{2}\boldsymbol{\gamma} R \boldsymbol{\gamma}] \equiv \exp\left[\tfrac{1}{2}\sum_{i,j=1}^{2N} \gamma_i R_{ij} \gamma_j\right], \tag{15a}$$

where R is a $2N\times 2N$ antisymmetrical matrix:

$$R = -\widetilde{R}, \qquad (\widetilde{R}_{ij} \equiv R_{ji}); \tag{15b}$$

in fact, if R had a symmetric part $S = \widetilde{S}$, $\boldsymbol{\gamma} S \boldsymbol{\gamma}$ would just be a c-number equal to $\frac{1}{2}\operatorname{Tr} S\sigma$, due to the commutation relations (11). The action (7) of $\mathscr{T}$ on the operators is easily shown to yield

$$\alpha_i = \mathscr{T}^{-1}\gamma_i \mathscr{T} = \sum_{j=1}^{2N} T_{ij}\gamma_j,$$

or

$$\boldsymbol{\alpha} = \mathscr{T}^{-1}\boldsymbol{\gamma}\mathscr{T} = T\boldsymbol{\gamma}, \tag{16}$$

where the $2N\times 2N$ matrix T is

$$T \equiv \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} = e^{\sigma R}. \tag{17}$$

The antisymmetry of R implies that T satisfies the condition

$$T\sigma\widetilde{T} = \sigma, \tag{18}$$

which simply means that the transformation (16) preserves the canonical commutation relation (11). Furthermore, the homomorphism

$$T' \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} T \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}$$

transforms (18) into $T'\tilde{T}' = 1$, so that the nonunitary linear transformations form a group, equivalent to the $2N\times 2N$ *complex orthogonal group*. The usual Bogoliubov group (which is equivalent to the $2N\times 2N$ real orthogonal group ([16])) is recovered if one restricts furthermore $\mathscr{T}$ to be unitary, or equivalently T' to be real, that is

$$T^* = \sigma T \sigma \;. \tag{19}$$

Boson case. Similarly, for bosons, we may write

$$\mathscr{T} = \exp[\boldsymbol{\lambda}\tau\boldsymbol{\gamma}]\exp[\tfrac{1}{2}\boldsymbol{\gamma}S\boldsymbol{\gamma}] \equiv \exp\left[\sum_{ij=1}^{2N}\lambda_i\tau_{ij}\gamma_j\right]\exp\left[\tfrac{1}{2}\sum_{ij}\gamma_i S_{ij}\gamma_j\right], \tag{20a}$$

where S is assumed without loss of generality to be symmetrical:

$$S = \tilde{S}\;; \tag{20b}$$

the linear form on operators $\boldsymbol{\gamma}$ in the first exponential has been noted for convenience $\boldsymbol{\lambda}\tau\boldsymbol{\gamma} \equiv \bar{\boldsymbol{c}}\cdot\boldsymbol{l}_1 - \boldsymbol{c}\cdot\boldsymbol{l}_2$, $\boldsymbol{\lambda}$ representing a set of $2N$ constants

$$\boldsymbol{\lambda} \equiv (\boldsymbol{l}_1, \boldsymbol{l}_2) \tag{20c}$$

($\boldsymbol{l}_1$ and $\boldsymbol{l}_2$ are N-dimensional vectors). The operators are transformed by (7) as

$$\alpha_i = \mathscr{T}^{-1}\gamma_i\mathscr{T} = \sum_{j=1}^{2N} T_{ij}\gamma_j + \lambda_i$$

or

$$\boldsymbol{\alpha} = \mathscr{T}^{-1}\boldsymbol{\gamma}\mathscr{T} = T\boldsymbol{\gamma} + \boldsymbol{\lambda}\;, \tag{21}$$

where the $2N\times 2N$ matrix

$$T \equiv \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} = e^{\tau S} \tag{22}$$

now satisfies the condition

$$T\tau\tilde{T} = \tau\;. \tag{23}$$

This again means that the transformation (21) preserves the commutation relations (13). The group of matrices T is now identified as the $2N\times 2N$ *complex symplectic group*. The usual unitary Bogoliubov group (equivalent to the real symplectic inhomogeneous group [17]) results by restricting T to satisfy (19), and $\boldsymbol{\lambda}$ to satisfy

$$l_1^* = l_2 \,. \tag{24}$$

Remarks. *a*) In (15) and (20), $\mathscr{T}$ has been expressed in terms of the operators $\boldsymbol{\gamma}$. It is easy to see that its expression in terms of the operators $\boldsymbol{\alpha}$ is exactly the same, since by use of (7)

$$\mathscr{T}\{\boldsymbol{\gamma}\} = \mathscr{T}^{-1}\times\mathscr{T}\{\boldsymbol{\gamma}\}\times\mathscr{T} = \mathscr{T}\{\mathscr{T}^{-1}\boldsymbol{\gamma}\mathscr{T}\} = \mathscr{T}\{\boldsymbol{\alpha}\}\,. \tag{25}$$

b) We shall not discuss the more difficult problem of constructing $\mathscr{T}$, once T is given. In particular, the group relations (18) or (23) do not necessarily ensure that T can be written in the exponential form (17) or (22); thus, in some peculiar cases, the $\mathscr{T}$ associated to a given T is not of the form (15) or (20). Moreover, in the boson case, if the parameters of T_{12} or T_{21} are too large, it may happen that the transformation $\mathscr{T}$ of eq. (20) has only a formal meaning, and that it takes the states out of the Hilbert space.

3. – Canonical decomposition of generalized Bogoliubov transformations.

Product of two fermion transformations. In general, the product $\mathscr{T}$ of two transformations $\mathscr{T}^{(1)}$ and $\mathscr{T}^{(2)}$ of the type (15) is also the exponential of a quadratic form, namely

$$\exp[\tfrac{1}{2}\boldsymbol{\gamma}R^{(1)}\boldsymbol{\gamma}]\exp[\tfrac{1}{2}\boldsymbol{\gamma}R^{(2)}\boldsymbol{\gamma}] = \exp[\tfrac{1}{2}\boldsymbol{\gamma}R\boldsymbol{\gamma}]\,, \tag{26a}$$

where $R^{(1)}$, $R^{(2)}$ and R are all antisymmetric, and satisfy

$$\exp[\sigma R^{(1)}]\exp[\sigma R^{(2)}] = \exp[\sigma R] \qquad \text{or} \qquad T^{(1)}T^{(2)} = T\,. \tag{26b}$$

Within a multiplicative constant, this result follows directly from (16) and (17). (This constant is 1 according to Haussdorf's theorem [18], which states that there exists a $\log\mathscr{T}$ in the Lie algebra of $\log\mathscr{T}^{(1)}$ and $\log\mathscr{T}^{(2)}$; here this Lie algebra contains only homogeneous antisymmetric quadratic forms.)

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[18] P. CARTIER: *Bull. Soc. Math. France*, **84**, 241 (1956).

Product of two boson transformations. A similar result holds for exponentials of *homogeneous* quadratic forms:

$$\exp[\tfrac{1}{2}\boldsymbol{\gamma}S^{(1)}\boldsymbol{\gamma}]\exp[\tfrac{1}{2}\boldsymbol{\gamma}S^{(2)}\boldsymbol{\gamma}]=\exp[\tfrac{1}{2}\boldsymbol{\gamma}S\boldsymbol{\gamma}]\,, \tag{27a}$$

where $S^{(1)}$, $S^{(2)}$, and S are symmetric, and satisfy

$$\exp[\tau S^{(1)}]\exp[\tau S^{(2)}]=\exp[\tau S] \qquad \text{or} \qquad T^{(1)}T^{(2)}=T\,. \tag{27b}$$

Multiplicative constants cannot however be eliminated for the *inhomogeneous* group. They already appear in the product of two « translations » $\boldsymbol{\gamma}\Rightarrow\boldsymbol{\gamma}+\boldsymbol{\lambda}$

$$\exp[\boldsymbol{\lambda}^{(1)}\tau\boldsymbol{\gamma}]\exp[\boldsymbol{\lambda}^{(2)}\tau\boldsymbol{\gamma}]=\exp[(\boldsymbol{\lambda}^{(1)}+\boldsymbol{\lambda}^{(2)})\tau\boldsymbol{\gamma}+\tfrac{1}{2}\boldsymbol{\lambda}^{(1)}\tau\boldsymbol{\lambda}^{(2)}]\,, \tag{28}$$

and also in

$$\exp[\boldsymbol{\lambda}\tau\boldsymbol{\gamma}]\exp[\tfrac{1}{2}\boldsymbol{\gamma}S\boldsymbol{\gamma}]=\exp[\tfrac{1}{2}\boldsymbol{\gamma}S\boldsymbol{\gamma}]\exp[\boldsymbol{\lambda}'\tau\boldsymbol{\gamma}]=\exp[\tfrac{1}{2}\boldsymbol{\gamma}S\boldsymbol{\gamma}+\boldsymbol{\mu}\tau\boldsymbol{\gamma}+\nu]\,, \tag{29a}$$

where

$$\boldsymbol{\lambda}=\exp[\tau S]\,, \qquad \boldsymbol{\lambda}'=\frac{\exp[\tau S]-1}{\tau S}\,\boldsymbol{\mu}\,, \tag{29b}$$

$$\nu=-\frac{1}{4}\boldsymbol{\lambda}\tau\,\frac{\operatorname{sh}\tau S-\tau S}{\operatorname{ch}\tau S-1}\,\boldsymbol{\lambda}\,. \tag{29c}$$

The formulae (27-29) are summarized in the general product law

$$\exp[\tfrac{1}{2}\boldsymbol{\gamma}S^{(1)}\boldsymbol{\gamma}+\boldsymbol{\lambda}^{(1)}\tau\boldsymbol{\gamma}]\exp[\tfrac{1}{2}\boldsymbol{\gamma}S^{(2)}\boldsymbol{\gamma}+\boldsymbol{\lambda}^{(2)}\tau\boldsymbol{\gamma}]=\exp[\tfrac{1}{2}\boldsymbol{\gamma}S\boldsymbol{\gamma}+\boldsymbol{\lambda}\tau\boldsymbol{\gamma}+\nu]\,, \tag{30a}$$

where

$$\exp[\tau S^{(1)}]\exp[\tau S^{(2)}]=\exp[\tau S]\,, \tag{30b}$$

$$\boldsymbol{\lambda}=\frac{\tau S}{\exp[\tau S]-1}\,\frac{\exp[\tau S^{(1)}]-1}{\tau S^{(1)}}\,\boldsymbol{\lambda}^{(1)}+\frac{\tau S}{1-\exp[-\tau S]}\,\frac{1-\exp[-\tau S^{(2)}]}{\tau S^{(2)}}\,\boldsymbol{\lambda}^{(2)}, \tag{30c}$$

$$\begin{aligned}\nu=\frac{1}{2}\boldsymbol{\lambda}^{(1)}\tau\,\frac{\operatorname{sh}\tau S^{(1)}-\tau S^{(1)}}{[\tau S^{(1)}]^2}\,\boldsymbol{\lambda}^{(1)}+\frac{1}{2}\boldsymbol{\lambda}^{(2)}\tau\,\frac{\operatorname{sh}\tau S^{(2)}-\tau S^{(2)}}{[\tau S^{(2)}]^2}\,\boldsymbol{\lambda}^{(2)}-\\ -\frac{1}{2}\boldsymbol{\lambda}\tau\,\frac{\operatorname{sh}\tau S-\tau S}{[\tau S]^2}\,\boldsymbol{\lambda}+\frac{1}{2}\boldsymbol{\lambda}^{(1)}\tau\,\frac{\exp[\tau S^{(1)}]-1}{\tau S^{(1)}}\,\frac{\exp[\tau S^{(2)}]-1}{\tau S^{(2)}}\,\boldsymbol{\lambda}^{(2)}\,.\end{aligned} \tag{30d}$$

The last term of ν exhibits the fact that the inhomogeneous Bogoliubov group can be represented in the Fock space only within multiplicative constants (phases in the unitary case).

Remark. These composition laws for bosons may be easily translated to linear transformations on oscillator co-ordinates $\{p_i, q_i\}$, by identifying q_i to $(c_i+\bar{c}_i)/\sqrt{2}$ and p_i to $i(\bar{c}_i-c_i)/\sqrt{2}$.

Some simple fermion transformations. Some of the nonunitary transformations introduced in Sect. **2** have a particularly simple effect. Let us consider three special types; we shall show in the following that they generate the most general transformation.

The first type is

$$\mathscr{T}^{(1)}\equiv\exp[\tfrac{1}{2}\,\bar{\boldsymbol{c}}X\bar{\boldsymbol{c}}]\equiv\exp\left[\tfrac{1}{2}\sum_{i,j=1}^{N}\bar{c}_iX_{ij}\bar{c}_j\right], \tag{31a}$$

where the $N\times N$ matrix X satisfies

$$\tilde{X}=-X\,. \tag{31b}$$

This transformation leaves the left vacuum ${}_c\langle\bar{0}|$ invariant. Its effect on the operators is, according to (16), (17):

$$\boldsymbol{\gamma}\Rightarrow[\mathscr{T}^{(1)}]^{-1}\boldsymbol{\gamma}\mathscr{T}^{(1)}=T^{(1)}\boldsymbol{\gamma}\,, \tag{32a}$$

$$T^{(1)}=\exp\left[\sigma\begin{pmatrix}0&0\\0&X\end{pmatrix}\right]=\begin{pmatrix}1&X\\0&1\end{pmatrix}, \tag{32b}$$

that is

$$\boldsymbol{c}\Rightarrow\boldsymbol{c}+X\bar{\boldsymbol{c}}\,,\qquad\bar{\boldsymbol{c}}\Rightarrow\bar{\boldsymbol{c}}\,, \tag{32c}$$

showing the invariance of the creation operators.

Similarly, the transformations of the type

$$\mathscr{T}^{(2)}\equiv\exp[\tfrac{1}{2}\boldsymbol{c}Z\boldsymbol{c}]\,, \tag{33a}$$

$$\tilde{Z}=-Z\,, \tag{33b}$$

leave the right vacuum $|0\rangle_c$ invariant. They transform the operators according to

$$\boldsymbol{\gamma}\Rightarrow[\mathscr{T}^{(2)}]^{-1}\boldsymbol{\gamma}\mathscr{T}^{(2)}=T^{(2)}\boldsymbol{\gamma}\,, \tag{34a}$$

$$T^{(2)}=\exp\left[\sigma\begin{pmatrix}Z&0\\0&0\end{pmatrix}\right]=\begin{pmatrix}1&0\\Z&1\end{pmatrix}, \tag{34b}$$

and do not modify the annihilation operators:

$$\boldsymbol{c}\Rightarrow\boldsymbol{c}\,,\qquad\bar{\boldsymbol{c}}\Rightarrow Z\boldsymbol{c}+\bar{\boldsymbol{c}}\,. \tag{34c}$$

The third type consists of « normal » transformations, which do not mix the creation to the annihilation operators. Their form is

$$\mathscr{T}^{(3)} \equiv \exp\left[\frac{1}{2}\Upsilon\begin{pmatrix}0 & -\tilde{Y}\\ Y & 0\end{pmatrix}\Upsilon\right] \equiv \exp[\bar{\boldsymbol{c}}Y\boldsymbol{c}]\exp[-\tfrac{1}{2}\operatorname{Tr}Y]\,. \tag{35}$$

Their only effect on both right and left vacuums is to multiply them by a constant. The operators transform according to

$$\boldsymbol{c} \Rightarrow e^{Y}\boldsymbol{c}\,, \qquad \bar{\boldsymbol{c}} \Rightarrow e^{-\tilde{Y}}\bar{\boldsymbol{c}}\,. \tag{36}$$

Canonical decomposition of a fermion transformation. It will now be shown that, in general, a transformation $\mathscr{T}$ of the form (15), (17) can be uniquely decomposed into the product

$$\mathscr{T} = \mathscr{T}^{(1)}\mathscr{T}^{(3)}\mathscr{T}^{(2)}\,, \tag{37a}$$

where $\mathscr{T}^{(1)}, \mathscr{T}^{(2)}, \mathscr{T}^{(3)}$ have respectively the forms (31), (33), (35), with

$$X = T_{12}(T_{22})^{-1}\,, \qquad Z = (T_{22})^{-1}T_{21}\,, \qquad e^{-Y} = \tilde{T}_{22}\,. \tag{37b}$$

(This decomposition is always possible provided $\det T_{22} \neq 0$.) The proof immediately follows from the product law (26), by an identification procedure:

$$T \equiv \begin{pmatrix}T_{11} & T_{12}\\ T_{21} & T_{22}\end{pmatrix} = \begin{pmatrix}1 & X\\ 0 & 1\end{pmatrix}\begin{pmatrix}e^{Y} & 0\\ 0 & e^{-\tilde{Y}}\end{pmatrix}\begin{pmatrix}1 & 0\\ Z & 1\end{pmatrix}. \tag{38}$$

The possibility of solving this eq. (38), as well as the antisymmetry (31*b*), (33*b*) of X and Z, are a consequence of the group law (18) satisfied by T. The interest of the canonical decomposition (37) lies in the fact that pairs of creation (annihilation) operators have been pushed out to the left (right).

Canonical decomposition of a boson transformation. An analogous scheme is followed for bosons, with two slight complications: linear forms have to be included in the exponentials, and constants arise from the product law (30). The three types of *special transformations* are now

$$\mathscr{T}^{(1)} \equiv \exp[\tfrac{1}{2}\bar{\boldsymbol{c}}X\bar{\boldsymbol{c}} + \boldsymbol{k}\cdot\bar{\boldsymbol{c}}]\,, \tag{39a}$$

$$X = \tilde{X} \tag{39b}$$

($\boldsymbol{k}$ being a N-dimensional vector), which transforms the operators as

$$\boldsymbol{c} \Rightarrow \boldsymbol{c} + X\bar{\boldsymbol{c}} + \boldsymbol{k}\,, \qquad \bar{\boldsymbol{c}} \Rightarrow \bar{\boldsymbol{c}}\,. \tag{39c}$$

Similarly, we introduce

$$\mathscr{T}^{(2)} \equiv \exp[\tfrac{1}{2}\boldsymbol{c}Z\boldsymbol{c} + \boldsymbol{k}'\cdot\boldsymbol{c}]\,, \tag{40a}$$

$$Z = \tilde{Z}\,, \tag{40b}$$

$$\boldsymbol{c} \Rightarrow \boldsymbol{c}\,, \qquad \bar{\boldsymbol{c}} \Rightarrow \bar{\boldsymbol{c}} - Z\boldsymbol{c} - \boldsymbol{k}'\,. \tag{40c}$$

Finally, the normal transformations are

$$\mathscr{T}^{(3)} \equiv \exp\left[\frac{1}{2}\gamma\begin{pmatrix}0 & \tilde{Y}\\ Y & 0\end{pmatrix}\gamma\right]e^{\nu} = \exp[\bar{\boldsymbol{c}}Y\boldsymbol{c}]\exp[\tfrac{1}{2}\operatorname{Tr}Y + \nu]\,, \tag{41a}$$

$$\boldsymbol{c} \Rightarrow e^{Y}\boldsymbol{c}\,, \qquad \bar{\boldsymbol{c}} \Rightarrow e^{-\tilde{Y}}\bar{\boldsymbol{c}}\,. \tag{41b}$$

With these definitions, $\mathscr{T}^{(1)}, \mathscr{T}^{(2)}$ and $\mathscr{T}^{(3)}$ have respectively the same actions on the right and left vacuums as the corresponding transformations for fermions.

The canonical decomposition of a general transformation $\mathscr{T}$ defined by (20), (22) is now obtained by use of (30), yielding

$$\mathscr{T} = \mathscr{T}^{(1)}\mathscr{T}^{(3)}\mathscr{T}^{(2)}\,, \tag{42a}$$

where the parameters of (39)-(41) are related to those of $T, \boldsymbol{\lambda}$ by

$$X = T_{12}[T_{22}]^{-1}\,, \qquad Z = -[T_{22}]^{-1}T_{21}\,, \qquad e^{-Y} = \tilde{T}_{22}\,, \tag{42b}$$

$$\boldsymbol{k} = \boldsymbol{l}_1 - X\boldsymbol{l}_2\,, \qquad \boldsymbol{k}' = -[T_{22}]^{-1}\boldsymbol{l}_2\,, \tag{42c}$$

$$\nu = \tfrac{1}{2}\boldsymbol{l}_2 X\boldsymbol{l}_2 - \tfrac{1}{2}\boldsymbol{l}_1\boldsymbol{l}_2\,. \tag{42d}$$

Here again quadratic and linear forms of creation operators have been pushed out to the left, and annihilation to the right, leaving in the middle a normal form with constants.

4. – Extension of Wick's theorem.

We now apply the formalism of nonunitary linear transformations (Sect. **2**) to the calculation of

$$\langle A\rangle_{ab} \equiv \frac{{}_a\langle 0|A|0\rangle_b}{{}_a\langle 0|0\rangle_b}\,. \tag{43}$$

In this expression A is an arbitrary operator, product of any number of creation and annihilation operators; $|0\rangle_a$ and $|0\rangle_b$ are two quasi-particle vacuums related to each other by a Bogoliubov transformation $\mathscr{T}$

$$|0\rangle_b = \mathscr{T}|0\rangle_a\,, \tag{44a}$$

where $\mathscr{T}$ is of the form (15) for fermions, or (20) for bosons. The operators $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, associated with $|0\rangle_a$ and $|0\rangle_b$, are related by eq. (16) or (21), *i.e.*

$$\boldsymbol{\alpha} = \mathscr{T}^{-1}\boldsymbol{\beta}\mathscr{T} = T\boldsymbol{\beta} \qquad \text{(fermions)}\,, \tag{44b}$$

$$\boldsymbol{\alpha} = \mathscr{T}^{-1}\boldsymbol{\beta}\mathscr{T} = T\boldsymbol{\beta} + \boldsymbol{\lambda} \qquad \text{(bosons)}\,. \tag{44c}$$

Moreover, $\mathscr{T}$ is unitary, and ${}_a\langle\bar{0}| = {}_a\langle 0|$, $\bar{a}_i = a_i^\dagger$ (the generalization to a non-unitary $\mathscr{T}$ is immediate but does not seem useful). In (43), we have divided the matrix-element of A by the overlap ${}_a\langle 0|0\rangle_b$ (assumed to be nonvanishing), in order to simplify the result of this paragraph. This overlap ${}_a\langle 0|0\rangle_b$ will be calculated explicitly in Sect. **5**.

Proof of the extended Wick's theorem. In order to evaluate (43), we shall now construct, by an appropriate linear nonunitary transformation, a new set of operators $\boldsymbol{\delta}$, such that each d_1 is a linear combination of the $\boldsymbol{b}$'s, and each $\bar{d}_i$ a linear combination of the $\boldsymbol{a}^\dagger$'s. Without restricting the generality of the method, we may choose for simplicity $\bar{d}_i = a_i^\dagger$; we therefore look for a $N\times N$ matrix W such that

$$\boldsymbol{d} \equiv W\boldsymbol{b}\,, \tag{45a}$$

$$\bar{\boldsymbol{d}} \equiv \boldsymbol{a}^\dagger \tag{45b}$$

satisfy the canonical (anti-) commutation relations. Relating by (44) the $a_i^\dagger$ to the $\{b_i, b_i^\dagger\}$, the only nontrivial condition

$$[d_i, \bar{d}_j]_\pm = \delta_{ij} \tag{46}$$

yields immediately, both for fermions and bosons,

$$W = [\tilde{T}_{22}]^{-1}\,, \tag{47}$$

provided T_{22} is nonsingular.

The elimination of the $\boldsymbol{b}$'s between (44) and (45) leads to the transformation

$$\boldsymbol{\alpha} = [\mathscr{T}^{(1)}]^{-1}\boldsymbol{\delta}\mathscr{T}^{(1)}\,, \tag{48}$$

which relates the set $\boldsymbol{\delta}$ to the set $\boldsymbol{\alpha}$. Namely, we get

$$\boldsymbol{a} = \boldsymbol{d} + X\bar{\boldsymbol{d}} \qquad \text{(fermions)}\,, \tag{49a}$$

$$\boldsymbol{a} = \boldsymbol{d} + X\bar{\boldsymbol{d}} + \boldsymbol{k} \qquad \text{(bosons)}\,, \tag{49b}$$

$$\boldsymbol{a}^\dagger = \bar{\boldsymbol{d}}\,, \tag{49c}$$

where

$$X = T_{12}[T_{22}]^{-1}\,, \tag{50a}$$

both for fermions and bosons, and where the N-dimensional vector $\boldsymbol{k}$ is for bosons

$$\boldsymbol{k} = \boldsymbol{l}_1 - X\boldsymbol{l}_2\,. \tag{50b}$$

Then, by use of eqs. (15)-(17) for fermions, (20)-(22) for bosons, we construct the corresponding operator $\mathscr{T}^{(1)}$ which relates the states. The result (in terms of the set $\boldsymbol{\alpha}$ by use of (25)) is

$$\mathscr{T}^{(1)} = \exp[\tfrac{1}{2}\boldsymbol{a}^\dagger X \boldsymbol{a}^\dagger] \qquad \text{(fermions)}\,, \tag{51a}$$

$$\mathscr{T}^{(1)} = \exp[\tfrac{1}{2}\boldsymbol{a}^\dagger X \boldsymbol{a}^\dagger + \boldsymbol{k}\cdot\boldsymbol{a}^\dagger] \quad \text{(bosons)}\,. \tag{51b}$$

The left vacuum ${}_d\langle\bar{0}|$ is then (eqs. (5′) and (51))

$${}_d\langle\bar{0}| = {}_a\langle 0|[\mathscr{T}^{(1)}]^{-1} = {}_a\langle 0|\,. \tag{52a}$$

The right vacuum $|0\rangle_d$, which from (45a) is proportional to $|0\rangle_b$, is (by use of the normalization condition (9b))

$$|0\rangle_d = |0\rangle_b[{}_a\langle 0|0\rangle_b]^{-1}\,. \tag{52b}$$

Consequently, $\langle A\rangle_{ab}$ takes now the simple form

$$\langle A\rangle_{ab} = {}_d\langle\bar{0}|A|0\rangle_d \tag{53}$$

of a « vacuum expectation value » in the bi-orthogonal bases associated to $\boldsymbol{\delta}$.

On the other hand, let us define now a normal product by writing the creation operators $\bar{d}_i$ on the left, and the annihilation operators d_i on the right (with the appropriate sign for fermions), and define the only nonvanishing contractions by

$$\overbrace{d_i\bar{d}_i} \equiv {}_d\langle\bar{0}|d_i\bar{d}_i|0\rangle_d = 1\,. \tag{54}$$

Any arbitrary product D of operators $\boldsymbol{\delta}$ is then equal to the sum of all the possible normal products with contractions, exactly like for the usual Wick's theorem. This result is obvious, since the proof of Wick's theorem ([9]) only involves the (anti-) commutation relations of the creation and annihilation operators, and not their property of being Hermitian conjugate. In particular, the « vacuum expectation value » ${}_d\langle\bar{0}|D|0\rangle_d$ is equal to the sum of all possible completely contracted products, as a result of the properties (9) of the right and left vacuums.

The creation and annihilation operators in A are linear combinations (inhomogeneous for bosons) of the operators $\boldsymbol{\delta}$. From the above considerations, and from eq. (53), it follows that $\langle A\rangle_{ab}$ is also equal to the sum of all possible completely contracted products (with the usual sign for fermions), in which appear contractions involving only a pair of operators (plus, for bosons, contractions of a single operator).

For instance, the potential energy is a sum of terms $\alpha_i\alpha_j\alpha_k\alpha_l$. Their matrix elements are, for fermions, equal to

$$(55a)\qquad {}_a\langle 0|\alpha_i\alpha_j\alpha_k\alpha_l|0\rangle_b=[{}_a\langle 0|0\rangle_b]^{-1}\{{}_a\langle 0|\alpha_i\alpha_j|0\rangle_b\,{}_a\langle 0|\alpha_k\alpha_l|0\rangle_b-\\ -{}_a\langle 0|\alpha_i\alpha_k|0\rangle_b\,{}_a\langle 0|\alpha_j\alpha_l|0\rangle_b+{}_a\langle 0|\alpha_i\alpha_l|0\rangle_b\,{}_a\langle 0|\alpha_j\alpha_k|0\rangle_b\}\;;$$

for bosons, re-expressing the contractions in terms of the one and two operator matrix elements, we get

$$(55b)\qquad {}_a\langle 0|\alpha_i\alpha_j\alpha_k\alpha_l|0\rangle_b=[{}_a\langle 0|0\rangle_b]^{-1}\{{}_a\langle 0|\alpha_i\alpha_j|0\rangle_b\,{}_a\langle 0|\alpha_k\alpha_l|0\rangle_b+\\ +{}_a\langle 0|\alpha_i\alpha_k|0\rangle_b\,{}_a\langle 0|\alpha_j\alpha_l|0\rangle_b+{}_a\langle 0|\alpha_i\alpha_l|0\rangle_b\,{}_a\langle 0|\alpha_j\alpha_k|0\rangle_b\}-\\ -2[{}_a\langle 0|0\rangle_b]^{-3}\,{}_a\langle 0|\alpha_i|0\rangle_b\,{}_a\langle 0|\alpha_j|0\rangle_b\,{}_a\langle 0|\alpha_k|0\rangle_b\,{}_a\langle 0|\alpha_l|0\rangle_b\,.$$

Explicit calculation of the contractions. If, for instance, A is expressed in terms of the operators $\boldsymbol{\alpha}$, the contractions are no longer 0 or 1 as in (54). Their explicit value is readily obtained by performing the transformation (49).

For *fermions*, only contractions of pairs appear. The nonvanishing ones are

$$(56a)\qquad \overline{a_i a_j}\equiv\langle a_i a_j\rangle_{ab}={}_d\langle\bar 0|a_i a_j|0\rangle_d=\\ ={}_d\langle\bar 0|\Big(d_i+\sum_m X_{im}\bar d_m\Big)\Big(d_j+\sum_n X_{jn}\bar d_n\Big)|0\rangle_d=X_{ji}=-\{T_{12}[T_{22}]^{-1}\}_{ij}\,,$$

$$(56b)\qquad \overline{a_i a_j^\dagger}\equiv\langle a_i a_j^\dagger\rangle_{ab}=\langle -a_j^\dagger a_i+\delta_{ij}\rangle_{ab}=\delta_{ij}\,,$$

summarized in matrix notation by

$$(56c)\qquad \overline{\boldsymbol{\alpha}\boldsymbol{\alpha}}=\begin{pmatrix}-T_{12}[T_{22}]^{-1} & 1\\ 0 & 0\end{pmatrix}.$$

If A is expressed in terms of the operators $\boldsymbol{\beta}$, we get through (16) and (18)

$$(57)\qquad \boldsymbol{\beta}=\sigma\tilde T\sigma\boldsymbol{\alpha}\,,$$

and hence

$$(58)\qquad \overline{\boldsymbol{\beta}\boldsymbol{\beta}}=\sigma\tilde T\sigma\,\overline{\boldsymbol{\alpha}\boldsymbol{\alpha}}\,\sigma T\sigma=\begin{pmatrix}0 & 1\\ 0 & -[T_{22}]^{-1}T_{21}\end{pmatrix}.$$

The mixed « contractions » $\overline{\boldsymbol{\alpha}\boldsymbol{\beta}}$ are particularly simple:

$$\overline{\boldsymbol{\alpha}\,\boldsymbol{\beta}} = \begin{pmatrix} 0 & [\widetilde{T}_{22}]^{-1} \\ 0 & 0 \end{pmatrix}. \tag{59}$$

For *bosons*, the inhomogeneity of the transformation $\boldsymbol{\delta} \Rightarrow \boldsymbol{\alpha}$ (eq. (49*b*)) also introduces single-operator contractions for the $\boldsymbol{\alpha}$:

$$\langle \boldsymbol{a} \rangle_{ab} = \boldsymbol{k} = \boldsymbol{l}_1 - T_{12}[T_{22}]^{-1}\boldsymbol{l}_2\,, \tag{60a}$$

$$\langle \boldsymbol{a}^\dagger \rangle_{ab} = 0\,. \tag{60b}$$

The calculation of pair contractions proceeds as for fermions:

$$\overline{a_i a_j} \equiv \langle a_i a_j \rangle_{ab} - \langle a_i \rangle_{ab} \langle a_j \rangle_{ab} = X_{ji} = \{T_{12}[T_{22}]^{-1}\}_{ij}\,, \tag{60c}$$

$$\overline{a_i a_j^\dagger} \equiv \langle a_i a_j^\dagger \rangle_{ab} - \langle a_i \rangle_{ab} \langle a_j^\dagger \rangle_{ab} = \delta_{ij}\,, \tag{60d}$$

or, in matrix form

$$\overline{\boldsymbol{\alpha}\boldsymbol{\alpha}} = \begin{pmatrix} T_{12}[T_{22}]^{-1} & 1 \\ 0 & 0 \end{pmatrix}. \tag{60e}$$

If A is expressed in terms of $\boldsymbol{\beta}$, the use of

$$\boldsymbol{\beta} = -\tau \widetilde{T} \tau (\boldsymbol{\alpha} - \boldsymbol{\lambda})\,, \tag{61}$$

which follows from (23) (44*c*), yields

$$\langle \boldsymbol{b} \rangle_{ab} = 0\,, \tag{62a}$$

$$\langle \boldsymbol{b}^\dagger \rangle_{ab} = -[T_{22}]^{-1}\boldsymbol{l}_2\,, \tag{62b}$$

$$\overline{\beta_i \beta_j} \equiv \langle \beta_i \beta_j \rangle_{ab} - \langle \beta_i \rangle_{ab} \langle \beta_j \rangle_{ab} = \begin{pmatrix} 0 & 1 \\ 0 & -[T_{22}]^{-1} T_{21} \end{pmatrix}_{ij}. \tag{62c}$$

The mixed contractions

$$\overline{\alpha_i \beta_j} \equiv \langle \alpha_i \beta_j \rangle_{ab} - \langle \alpha_i \rangle_{ab} \langle \beta_j \rangle_{ab}\,, \tag{63}$$

are also given by eq. (59).

Remark. This extension of Wick's theorem has been proved under two conditions: we assumed from the beginning that the two vacuums $|0\rangle_a$ and $|0\rangle_b$

were not orthogonal, in order to define $\langle A\rangle_{ab}$; furthermore, we needed T_{22} not to be singular (*i.e.* $\det T_{22} \neq 0$), to construct the set of operators $\boldsymbol{\delta}$. In Sect. **5**, it will be shown that these two conditions are equivalent for fermions (eq. (66)), and that both are always satisfied for bosons (eqs. (67), (68)).

5. – Explicit calculation of the overlap. Discussion.

In order to achieve the explicit calculation of a matrix element ${}_a\langle 0|A|0\rangle_b$, we need to express the overlap ${}_a\langle 0|0\rangle_b$ in terms of the parameters of the transformation $\mathscr{T}$ which relates $\boldsymbol{\beta}$ to $\boldsymbol{\alpha}$ (eq. (44)). This result will follow immediately from the application of the decomposition (37) or (42) of Sect. **3** to this transformation $\mathscr{T}$.

We first notice that the transformation $\mathscr{T}^{(1)}$ introduced in Sect. **4** to construct the set $\boldsymbol{\delta}$ (eqs. (48)-(51)) is precisely the first factor of this canonical decomposition of $\mathscr{T}$ (eqs. (31), (37*b*) for fermions or eqs. (39), (42*b*), (42*c*) for bosons). The set of operators $\boldsymbol{\delta}$ thus appears as intermediate between $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$.

From eq. (44*a*), this overlap is

$$(64) \qquad {}_a\langle 0|0\rangle_b = {}_a\langle 0|\mathscr{T}|0\rangle_a\,,$$

where $\mathscr{T}$ is expressed in terms of the operators $\boldsymbol{\alpha}$ (eq. (25)). The use of (37) or (42) gives

$$(65) \qquad {}_a\langle 0|0\rangle_b = {}_a\langle 0|\mathscr{T}^{(1)}\mathscr{T}^{(3)}\mathscr{T}^{(2)}|0\rangle_a = {}_a\langle 0|\mathscr{T}^{(3)}|0\rangle_a\,,$$

as a consequence of the simple action of $\mathscr{T}^{(1)}$ and $\mathscr{T}^{(2)}$. For *fermions*, eq. (65) with the help of (35), (37*b*) reduces to

$$(66) \qquad {}_a\langle 0|0\rangle_b = [\det T_{22}]^{\frac{1}{2}}\,.$$

For *bosons*, eq. (65), together with (41) and (42*b*), (42*d*), becomes

$$(67) \qquad {}_a\langle 0|0\rangle_b = [\det T_{22}]^{-\frac{1}{2}} \exp\left[\tfrac{1}{2}\boldsymbol{l}_2 T_{12}[T_{22}]^{-1}\boldsymbol{l}_2 - \tfrac{1}{2}\boldsymbol{l}_1\cdot\boldsymbol{l}_2\right].$$

Validity of the extension of Wick's theorem. For *fermions*, the explicit evaluation (66) of the overlap ${}_a\langle 0|0\rangle_b$ shows that the two conditions ${}_a\langle 0|0\rangle_b \neq 0$ and $\det T_{22} \neq 0$, which needed to be assumed in the derivation of this theorem, are equivalent. Therefore, the only condition of validity is that the two vacuums are not orthogonal. (Any vacuum $|0\rangle_b$ orthogonal to $|0\rangle_a$ results from $|0\rangle_a$ by exciting quasi-particles, as may be seen from the decomposition of $\mathscr{T}$ given in ref. ([16]).)

For bosons, it is easy to see that T_{22} is never singular, as a consequence of the unitarity of $\mathscr{T}$. The unitarity condition (19) together with the group property (23) imply in particular

$$T_{22}T_{22}^{\dagger} = 1 + T_{21}T_{21}^{\dagger} .$$

The Hermitian matrix $T_2 T_2^{\dagger}$ has therefore all its eigenvalues larger than 1, or equal to 1 if $T_{21} = 0$. (In fact, these eigenvalues are precisely the $|u_k|^2 = 1 + |v_k|^2$ of the standard decomposition of $\mathscr{T}$, given in ref. [17].) Consequently, we get

$$|\det T_{22}| \geqslant 1 . \tag{68}$$

On the other hand, from (67), it is obvious that ${}_a\langle 0|0\rangle_b \neq 0$, provided the number of single-particle states is finite. Thus, if two boson vacuums $|0\rangle_a$ and $|0\rangle_b$ are unitarily related by a Bogoliubov transformation their overlap never vanishes, and the extension of Wick's theorem is always valid.

Further extension to nonzero temperature. Another generalization of Wick's theorem, commonly used in statistical mechanics [19], applies to thermal averages

$$\frac{\operatorname{Tr}\exp[-\beta Q]A}{\operatorname{Tr}\exp[-\beta Q]} \tag{69}$$

where Q is some Hermitian quadratic form of the operators $\boldsymbol{\alpha}$ (plus linear terms for bosons). This result will now be extended to a non-Hermitian Q. First, through an appropriate nonunitary transformation (15), (16) or (20), (21) on the operator algebra, Q becomes

$$Q = \sum_i q_i \tilde{d}_i d_i + r , \tag{70}$$

(where we assume $\operatorname{Re} q_i \geqslant 0$). Then, if the quantity (69) is expressed (through (70) and the closure relation (6)) on the biorthogonal bases (3′), (5′) associated to the set $\boldsymbol{\delta}$, Gaudin's derivation [19] applies without change, since again it is based only on the commutation relations.

The fact that Wick's theorem may be extended to (69), with a non-Hermitian Q, also appears as a « nonzero temperature » generalization of the theorem proved in Sect. **3**: in fact, the vacuum expectation value (43), (53) is recovered

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[19] M. GAUDIN: *Nucl. Phys.*, **15**, 89 (1960).

as the zero-temperature limit of (69), since

$$\lim_{\beta\to\infty}\frac{\operatorname{Tr}\exp[-\beta Q]A}{\operatorname{Tr}\exp[-\beta Q]}={}_{d}\langle\bar{0}|A|0\rangle_{d}=\langle A\rangle_{ab}\,.$$

* * *

We wish to thank G. Ripka for stimulating discussions.

RIASSUNTO (*)

Si considerano trasformazioni lineari, che conservano le regole di (anti) commutazione, ma non la relazione di ermiticità, per gli operatori di creazione e distruzione dei bosoni (fermioni); queste trasformazioni portano alle rappresentazioni dello spazio di Fock sulle basi biortogonali dell'algebra degli operatori. Come applicazione, si ricava un'estensione del teorema di Wick agli elementi di matrice di un operatore arnitrario fra due differenti vuoti di quasi particelle. Questo teorema è utile per calcoli che vanno al di là dei metodi variazionali di Hartree-Fock-Bogoliubov (H.F.B. con proiezione, metodo delle coordinate del generatore, ecc.). Si stabilisce una decomposizione canonica per trasformazioni di Bogoliubov, che si dimostra utile per esempio nel calcolo della sovrapposizione dei differenti vuoti di due particelle.

(*) *Traduzione a cura della Redazione.*

Неунитарные преобразования Боголюбова и обобщение теоремы Вика.

Резюме (*). — Рассматриваются линейные преобразования, которые сохраняют (анти-) коммутационные правила, но не соотношение эрмитовости для (фермионных) бозонных операторов рождения и уничтожения; эти преобразования приводят к пространственным представлениям Фока на биортогональных базисах алгебры операторов. Как иллюстрация, выводится обобщение теоремы Вика для матричных элементов произвольного оператора между двумя различными квази-частичными вакуумами. Эта теорема оказывается полезной для вычислений, которые выходят за рамки вариационных методов Хартри-Фока-Боголюбова (метод Х-Ф-Б с проектированием, генераторный координатный метод и др.). Устанавливается каноническое разложение для преобразований Боголюбова, которое оказывается полезным, например, при вычислении перекрытия двух различных квази-частичных вакуумов.

(*) *Переведено редакцией.*