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Section A :
Physique théorique.

Translation invariant quasi-free states and Bogoliubov transformations

by

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ABSTRACT. — Bogoliubov transformations acting as permutations of translation invariant quasi-free states of fermions are precisely defined and studied. In particular the orbits and stabilizers are completely classified. In the case of pure states connections to previous related results are given.

INTRODUCTION

Bogoliubov transformations are widely used in many physical problems and specially in connection to Hartree-Fock approximation. It is known that in general such transformations are not unitarily implemented but merely define in general new representations of the Clifford algebra. Now if one considers for instance the central state, then from its uniqueness it is clear that it is invariant under any automorphism acting by duality. So that it seems interesting to classify the orbits of the Bogoliubov transformations within the set of quasi-free states. We accomplish this program in the case of translation invariant quasi-free states and show that the orbits are completely defined by a L_∞ function. We give explicitly the Bogoliubov transformation connecting two states in the same orbit.

The proofs are simplified by a particular representation of the mono-

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particular space which allows a new description of the group of Bogoliubov transformations as functions in U_2.

The last section is specially devoted to pure states which correspond to complexifications of the monoparticular space. We establish the connection of our results with the theorem (see [1]) which states that any two pure states are connected by a generalized Bogoliubov transformation not necessarily commuting with translations.

I. NOTATIONS AND DEFINITIONS

We shall not repeat in this section all definitions and results already known about quasi-free states over the C*-algebra of anticommutation relations, but only the main points which will be used in the sequel. We shall refer to [1] for more details.

a) One particle space.

$\mathcal{A}$ will be the Clifford algebra built over the one particle space of square integrable functions of impulsion; the fundamental symmetric form s will be the real part of the ordinary scalar product of this one particle space $h = \mathcal{L}_2(\mathrm{R}^3)$. A complex structure on h is defined by a R-linear operator J satisfying

$$J^+ = -J, \qquad J^2 = -1$$

In [1] it is shown that it is possible to find a R-linear symmetric involution Λ anticommuting with J.

A particular choice of J is the multiplication by i and for Λ the usual operation:

$$(1) \qquad \Lambda\psi(p) = \overline{\psi(-p)} = \psi^v(p) \qquad \psi \in \mathcal{L}_2(\mathrm{R}^3)$$

This choice is natural if we want to study translation invariant states and monoparticular transformations commuting with translations; later on we shall come back to other possible choices and to their implications (see last section). Indeed it is well known that any R-linear operator A on h which commutes with translations can be written:

$$(2) \qquad A\psi(p) = A_1(p)\psi(p) + A_2(p)\psi^v(p)$$

where $p \to A_i(p)$ $(i = 1, 2)$, are L_∞ functions.

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[1] E. Balslev, J. Manuceau and A. Verbeure, *Comm. Math. Phys.*, t. 8, 1968, p. 315.

Let us now emphasize a trick which will be of main importance for the simplification of the proofs. One can identify in a natural way the real space h with the graph of Λ, considered as a real space, $\mathcal{H}$:

$$\psi \in h \to \frac{1}{\sqrt{2}}(\psi, \Lambda\psi) \in \mathcal{H}$$

Clearly this correspondence is isometric with respect to the restriction to $\mathcal{H}$ of the real scalar product on $h \times h$

$$((\psi, \varphi), (\psi', \varphi')) = s(\psi, \varphi) + s(\psi', \varphi')$$

In this scheme a R-linear operator A commuting with translations is identified (see (2)) to L_∞ functions into 2×2 complex matrices acting by pointwise ordinary multiplication on $\mathcal{H}$:

$$p \to \begin{pmatrix} A_1(p) & A_2(p) \\ \overline{A}{}_2^\vee(p) & \overline{A}{}_1^\vee(p) \end{pmatrix} \tag{3}$$

This identification respects the algebraic structure of operators in h: multiplication of operators on h corresponds to pointwise ordinary matrix multiplication, adjonction in h with respect to the real scalar product to pointwise adjunction:

$$\begin{pmatrix} A_1 & A_2 \\ \overline{A}{}_2^\vee & \overline{A}{}_1^\vee \end{pmatrix}^+ = \begin{pmatrix} \overline{A}_1 & A_2^\vee \\ \overline{A}_2 & A_1^\vee \end{pmatrix} \tag{4}$$

b) Quasi-free states.

It is shown in [*1*] that any R-linear operator A satisfying

$$A^+ = -A \tag{5}$$

$$\| A \| \leqslant 1 \tag{6}$$

uniquely defines a quasi-free state ω_A over $\mathcal{A}$, and conversely, by the relation:

$$\omega_A(B(\psi)B(\varphi)) = s(\psi, \varphi) + is(A\psi, \varphi) \tag{7}$$

If translation invariance is requested, in our description the relation (5) reads:

$$\overline{A}_1(p) = -A_1(p) \quad , \quad A_2^\vee(p) = -A_2(p) \tag{8}$$

almost everywhere (up to now such a restriction will not be repeated if no confusion is possible).

We shall say that ω_A, translation invariant, is gauge invariant if $A_2 = 0$. The inequality (6) will be reexpressed later (cf. (21)).

c) Bogoliubov transformations.

In an abstract way we define Bogoliubov transformations as *-automorphisms of $\mathcal{A}$ commuting with translations and induced by one particle transformations.

This definition coincides with the usual one; indeed via the previous remarks on one particle transformations in h it is obvious that the group $\mathcal{B}$ of such automorphisms is isomorphic to a subgroup of L_∞ functions in U_2

$$p \to \begin{pmatrix} u(p) & v(p) \\ \bar{v}^{\vee}(p) & \bar{u}^{\vee}(p) \end{pmatrix}$$

with pointwise multiplication and inversion.

Orthogonality of the corresponding one particle transformation U:

$$UU^+ = U^+U = 1$$

implies the set of well known relations:

$$(9) \qquad |u|^2 + |v|^2 = 1 \quad , \quad u^{\vee}v + uv^{\vee} = 0$$

$$(10) \qquad |u|^2 + |v^{\vee}|^2 = 1 \quad , \quad \bar{u}v + \bar{u}^{\vee}v^{\vee} = 0$$

Actually one set of relations is needed; the other can be then deduced. Using previous relations one can easily see that the group $\mathcal{B}$ is isomorphic to the set of L_∞ functions in U_2

$$(11) \qquad p \to e^{i\varepsilon(p)}\begin{pmatrix} u(p) & v(p) \\ -\bar{v}(p) & \bar{u}(p) \end{pmatrix}$$

with

$$(12) \qquad \varepsilon = -\varepsilon^{\vee} = \bar{\varepsilon}$$

$$(13) \qquad u = u^{\vee}$$

$$(14) \qquad v = -v^{\vee}$$

In this special representation the center of $\mathcal{B}$ appears as the subgroup of elements

$$p \rightarrow \begin{pmatrix} e^{i\varepsilon(p)} & 0 \\ 0 & e^{i\varepsilon(p)} \end{pmatrix} \tag{15}$$

II. BOGOLIUBOV TRANSFORMATIONS OF QUASI-FREE STATES

a) Transformations of quasi-free states induced by Bogoliubov transformations.

Let ω be a state on $\mathcal{A}$ and τ a *-automorphism of $\mathcal{A}$. One defines by duality the state ω_τ on $\mathcal{A}$ as

$$\omega_\tau(X) = \omega(\tau(X)) = \{ \omega \circ \tau \} (X), \qquad \forall X \in \mathcal{A} \tag{16}$$

Let $\mathfrak{J}$ be the set of translation invariant quasi-free states and $\tau \in \mathcal{B}$; then τ leaves $\mathfrak{J}$ invariant as a whole.

It is clear that if $\omega = \omega_A \in \mathfrak{J}$, we have $\omega_\tau = \omega_{A'}, \in \mathfrak{J}$ with

$$A' = U^+AU \tag{17}$$

where U is the one particle transformation which corresponds to τ. The translation invariance allows to rewrite (17) as:

$$A_1' = | u |^2(A_1 + A_1^\vee) - A_1^\vee - \overline{uv}A_2 + uv\overline{A}_2 \tag{18a}$$

$$A_2' = u\bar{v}(A_1 + A_1^\vee) + \bar{u}^2 A_2 + v^2 \overline{A}_2 \tag{18b}$$

We used the identification of A and U with matrices in $\mathcal{H}$ and also formulas (8), (13) and (14).

We shall call orbit associated with $\omega_{A'} \in \mathfrak{J}$ the set of ω_A such that ω_A and $\omega_{A'}$ are connected by a Bogoliubov transformation acting by duality as in (16).

Up to this point it is necessary to emphasize on a class of invariant quasi-free states: the $\mathcal{B}$-invariant quasi-free states.

b) $\mathcal{B}$-invariant quasi-free states.

Definition: a translation invariant quasi-free state ω_A will be called $\mathcal{B}$-invariant if

$$A_1 + A_1^\vee = 0 \quad , \quad A_2 = 0 \tag{19}$$

It is obvious, by the formulas (18) that these states are invariant under any Bogoliubov transformation. Conversely, if a quasi-free state is invariant under all Bogoliubov transformations, then it satisfies both previous relations. The proof lies in the fact that a Bogoliubov transformation acts on $A_1 + A_1^{\vee}$, A_2 and $\overline{A}_2$ as a linear transformation which cannot be singular for every U.

Let us remark that if A is $\mathcal{B}$-invariant, then

$$A = a.1 \qquad a \in L_\infty \tag{20}$$

where 1 is the identity in $\mathcal{H}$ and $a^{\vee} = \bar{a} = -a$; the proof is evident. We shall see later another characterization of $\mathcal{B}$-invariant states but turn now to the central problem which is the study of the orbits of $\mathcal{B}$ in $\mathfrak{I}$.

c) Classification of the orbits.

Up to now, we did not use the condition (6) on A. This can be reformulated here as (see [*1*]):

$$X^2 = 1 - i(A_1 - A_1^{\vee}) + A_1 A_1^{\vee} - | A_2 |^2 \geqslant 0 \tag{21}$$

Let us now introduce somewhat symbolic notations; we define the L_∞ functions (cf. (3) and (8)):

$$\mathrm{Tr}_{\mathcal{H}}(A) = A_1 - A_1^{\vee} \tag{22}$$

$$\mathrm{Det}_{\mathcal{H}}(A) = A_1 A_1^{\vee} - | A_2 |^2 \tag{23}$$

so that (21) can be rewritten as:

$$X^2 = \mathrm{Det}_{\mathcal{H}}(1 - iA) \tag{24}$$

LEMMA 1. — X^2 *is invariant through a Bogoliubov transformation.*

The formula (24) makes the lemma evident through the formula (17) and elementary properties of matrix conjugation.

Actually both $\mathrm{Det}_{\mathcal{H}}(A)$ and $\mathrm{Tr}_{\mathcal{H}}(A)$ are invariant and they are the only invariants of $A.X^2$ gathers both of them since:

$$2i\, \mathrm{Tr}_{\mathcal{H}}(A) = X^2 - X^{2^{\vee}} \tag{25}$$

$$-2\, \mathrm{Det}_{\mathcal{H}}(A) = 1 + X^2 + X^{2^{\vee}} \tag{26}$$

LEMMA 2. — *The condition*

$$\sqrt{X^2} + \sqrt{X^{2\vee}} = 2 \tag{27}$$

is necessary and sufficient in order that the corresponding quasi-free state be $\mathcal{B}$-invariant.

The necessity follows from (19) and (21); the converse is proved by an elementary calculation: using explicit expression for X^2 one obtains that (27) is equivalent to

$$|A_1 + A_1^\vee|^2 + 4|A_2|^2 = 0 \tag{28}$$

which proves the lemma.

LEMMA 3. — *Any orbit contains at least a gauge invariant state.*

Let ω_A a quasi-free state and Δ_0 the symmetric domain (*i. e.* the Lebesgue measure of the symmetric difference between Δ_0 and $-\Delta_0$ is zero) where:

$$\sqrt{X(p)^2} + \sqrt{X^\vee(p)^2} = 2 \qquad p \in \Delta_0$$

and Δ_1 the complementary set of Δ_0. We give explicitly a Bogoliubov transformation which connects ω_A to $\omega_{A'}$ such that $A_2' = 0$:

$$u(p) = 1 \quad \text{and} \quad v(p) = 0, \qquad \text{for } p \in \Delta_0 \tag{29}$$

and for $p \in \Delta_1$

$$\begin{aligned} u &= \frac{A_1 + A_1^\vee}{|A_1 + A_1^\vee|}\sqrt{\frac{1+\alpha}{2}} \\ v &= \frac{A_2}{|A_2|}\sqrt{\frac{1-\alpha}{2}} \end{aligned} \tag{30}$$

with

$$\alpha = \alpha^\vee = \frac{|A_1 + A_1^\vee|}{\sqrt{|A_1 + A_1^\vee|^2 + 4|A_2|^2}} \leqslant 1 \tag{31}$$

In the case where $A_1 + A_1^\vee = 0$ and $A_2 \neq 0$, one can choose:

$$\begin{aligned} u &= \frac{i}{\sqrt{2}} \\ v &= \frac{A_2}{\sqrt{2}\,|A_2|} \end{aligned} \tag{32}$$

One should realize that the previous lemma is essentially the fact that an antihermitian matrix can be diagonalized by a unitary transformation. Actually, the solution given is not unique as we shall see; two solutions differ by an element of the stabilizer of $\omega_{A'}$ (1) which will be studied later.

LEMMA 4. — *Two gauge invariant states can be connected by an element of $\mathcal{B}$ if and only if they have the same* X^2.

The last part is evident by the Lemma 1. Conversely, let ω_A and $\omega_{A'}$ such that $X^2 = X'^2$; this gives two relations:

$$A_1 - \check{A}_1 - A_1' + \check{A}_1' = 0 \quad , \quad A_1\check{A}_1 - A_1'\check{A}_1' = 0$$

which are equivalent to

$$(A_1 - A_1')(A_1 + \check{A}_1') = 0 \tag{33}$$

so that on a domain $\Delta_+ \subset R^3$

$$A_1(p) = A_1'(p) \qquad p \in \Delta_+$$

Clearly, Δ_+ is a symmetric domain and in the same way it exists a symmetric domain Δ_- such that

$$A_1(p) = -\check{A}_1'(p) \qquad p \in \Delta_-$$

According to these results and formulas (18), one can choose as Bogoliubov transformation connecting ω_A and $\omega_{A'}$, the automorphism given by:

$$\begin{array}{llll} u(p) = 1 & \text{and} \quad v(p) = 0 & \text{for} & p \in \Delta_+ \\ u(p) = 0 & \text{and} \quad v(p) = 1 & \text{for} & p \in \Delta_- \end{array} \tag{34}$$

It is easy to see that, up to a set of zero Lebesgue measure, we have:

$$\Delta_+ \cup \Delta_- = R^3$$

and that, on $\Delta_+ \cap \Delta_-$, $\omega_A = \omega_{A'}$ is a $\mathcal{B}$-invariant state, so that u and v can be chosen arbitrarily in this domain.

All the previous results are gathered in the following proposition:

PROPOSITION 1. — *The function* X^2 *gives a complete characterization of the orbits of* $\mathcal{B}$ *in* $\mathfrak{I}$. *If*

i) $\sqrt{X^2} + \sqrt{\check{X^2}} = 2$, *the orbit reduces to a point,*

(1) The stabilizer of ω_A is defined by : $\mathcal{B}_A = \{ \tau \in \mathcal{B} \, ; \, \omega_A \circ \tau = \omega_A \}$.

ii) $\sqrt{X^2} + \sqrt{X^{2\nu}} \neq 2$ *at least on a domain of non zero measure; then the orbit contains an infinity of points ; an infinite subfamily of which is gauge invariant.*

PROPOSITION 2. — $\mathfrak{J}$ *contains an infinity of layers* (1) *with respect to* $\mathfrak{B}$, *indexed by a symmetric domain* $\Delta_0 \subset R^3$.

Proof. — Let Δ_0 be the set of points in R^3 where

$$\sqrt{X^2(p)} + \sqrt{X^{2\nu}(p)} = 2 \qquad p \in \Delta_0$$

for a given state and let $\mathfrak{B}_A$ the stabilizer of this state ω_A. Then as we saw previously there is no restriction for the elements of $\mathfrak{B}_A$ on the domain Δ_0. In $\Delta = \complement\Delta_0$ (up to a set of zero measure) there is in the orbit of ω_A a point which is gauge invariant ω_{A^0}. Any element of $\mathfrak{B}_{A^0}$ is restricted to correspond to

$$u(p) = \exp(i\Omega(p)) \quad \text{and} \quad v(p) = 0 \qquad p \in \Delta \tag{35}$$

a form which actually does not depend of X^2. Using the well known fact that along an orbit stabilizers are the same up to a conjugation, we get the result.

The formula (35) is easily deduced from (18) for instance, restricted to $A_2 = 0$.

For sake of completeness, let us give a result which brings some insight in the structure of $\mathfrak{B}$.

PROPOSITION 3. — *The intersection of stabilizers is exactly the center of* $\mathfrak{B}$.

Proof. — It is evident from formulas (15) and (18) that the center $C(\mathfrak{B})$ of $\mathfrak{B}$ is included in the intersection $\bigcap_A \mathfrak{B}_A$ of stabilizers. On the other hand, let $\tau \in \bigcap_A \mathfrak{B}_A$, τ is certainly given by :

$$u = \exp(i\Omega) \quad \text{and} \quad v = 0 \tag{36}$$

since it belongs at least to the stabilizer of one gauge invariant state and the conclusion results of previous characterization of the center of $\mathfrak{B}$ (see (15)).

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(1) We define the layers in J with respect to $\mathfrak{B}$ as the sets of elements of J the stabilizers of which are conjugated within $\mathfrak{B}$.

It is clear by definition that the subgroup $C(\mathcal{B})$ contains as a special case the subgroup of translation *-automorphisms, of which $C(\mathcal{B})$ is in a certain sense the generalization.

Up to this point, the classification of translation invariant quasi-free states into orbits with respect to $\mathcal{B}$ is complete; in the next paragraph we shall consider in more details the pure states, which correspond to complexifications, and show explicitly how they split in orbits.

III. COMPLEXIFICATIONS AND CONJUGATIONS

At the very beginning we chose in the one particle space h both a particular complexification J_0 (the multiplication by i) and a special conjugation Λ_0 (complex conjugation). Later on, we shall need other possibilities; so it is our aim to describe all other possibilities. As any two complexifications are linked through a one particle transformation (in general not commuting with translations: see [*1*]) we can separately consider possible choices of Λ for given J (say J_0) and later change J. For the first part, the next lemma shows that Λ is almost uniquely determined by J.

LEMMA 5. — *Any symmetric involution commuting with translations and anticommuting with* J_0 *is in* $\mathcal{H}$ *of the form*

$$(37) \qquad \Lambda = \begin{pmatrix} 0 & e^{i\varepsilon} \\ e^{-i\varepsilon} & 0 \end{pmatrix}$$

with $\varepsilon = \bar{\varepsilon} = \varepsilon^{\vee}$.

Proof. — Λ_0 is defined as

$$\Lambda_0\psi = \overline{\psi}^{\vee} \qquad \psi \in \mathcal{L}_2(\mathrm{R}^3)$$

and clearly $\Lambda_0\Lambda$ is a C-linear operator commuting with translations so that it can be written

$$\Lambda_0\Lambda\psi = a\psi \qquad \text{where} \qquad a \in \mathrm{L}_\infty$$

so that

$$(38) \qquad \Lambda\psi = \bar{a}^{\vee}\overline{\psi}$$

The fact that $\Lambda = \Lambda^+$ and $\Lambda^2 = 1$ implies $\bar{a}^{\vee}a = 1$ and $a^{\vee} = a$. Λ so defined is connected to Λ_0 by a Bogoliubov transformation. Now let us come back to complexifications; a complete classification with respect to Bogoliubov transformations is given by the following lemma:

LEMMA 6. — *Different complexifications split into orbits with respect to Bogoliubov transformations, characterized by a symmetric domain* $\Delta_0 \subset R^3$; *the orbit defined by* J_0 *corresponds to* Δ_0 *of zero Lebesgue measure.*

Proof. — Let J be a complexification commuting with translations

$$J\psi = J_1\psi + J_2\bar{\psi}^{\vee} \quad , \quad \psi \subset \mathcal{L}_2(R^3)$$

It is easy to verify that J_1 and J_2 satisfy

$$J_1^2 - |J_2|^2 = -1 \quad , \quad J_2(J_1 - J_1^{\vee}) = 0$$

so that within a symmetric domain $\Delta_1 \subset R^3$

$$J_1(p) = J_1^{\vee}(p) \qquad p \in \Delta_1 \tag{39}$$

and on this domain J is connected to J_0 by a Bogoliubov transformation. On the complementary domain Δ_0 of Δ_1

$$J_1(p) = -J_1^{\vee}(p) = \pm i \tag{40}$$

so that $J_2(p) = 0$ and it is a $\mathcal{B}$-invariant complexification.

Such a situation is completely described by the following lemma :

LEMMA 7. — *A* $\mathcal{B}$*-invariant complexification* J_i *on* $\Delta_0 \subset R^3$ *is determined by a splitting of* Δ_0 *into two parts such that*

$$p \in \Delta_0^+ \Leftrightarrow -p \in \Delta_0^-$$

and

$$J_i\psi = i\psi^+ - i\psi^- \qquad \text{wehre} \qquad \psi^\pm = \psi/\Delta_0^\pm$$

The proof is evident from the previous calculations.

One can realize that the orthogonal operator T which links J_i to J_0 is given by

$$T\psi = \psi^+ + \bar{\psi}^- \qquad \psi \in \mathcal{L}_2(R^3) \tag{41}$$

and satisfies

$$T^+ = T^{-1} = T \quad , \quad T^+J_0T = J_i$$

It is clear that this operator does not commute with translations.

Using this explicit form of T one can deduce (this can also be done explicitly) that a corresponding conjugation is for instance

$$\Lambda = T^{+}\Lambda_0 T$$

which gives

$$\Lambda\psi = \psi^{\vee} \qquad \psi \in \mathcal{L}_2(R^3) \tag{42}$$

and therefore does not commute with translations. Indeed this last fact is to be expected since J_i belongs to the center of $\mathcal{B}$.

I . CONCLUSION

In this paper we have given a description as complete as possible of the action induced on translation invariant quasi-free states by one particle transformations commuting with translations. The translation invariance of Bogoliubov transformations is certainly a restriction as it is known already and explicitly shown in the last section where different orbits gather when the group is enlarged to one particle transformations not commuting with translations. Nevertheless this definition Bogoliubov of transformation coincide with the familiar one and one has to realize that the special representation of the one particle space is actually well fitted to the translation invariant case.

On the other hand, if we disregard states which are not invariant by reflexions in the Fourier space, the results are simplified and for instance pure states belong to a unique orbit. The importance of this invariance, which is usually assumed in models, will be studied in a forthcoming paper, which will be devoted to possible evolutions linked to quasi-free states under the K. M. S. boundary conditions and where we shall use the results of this work in the translation invariant case.

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