NUCLEAR THEORY, Vol. 40 (2023)
eds. M. Gaidarov, N. Minkov, Heron Press, Sofia

"Onishi" Formulas

K. Neergård

Fjordtoften 17, 4700 Næstved, Denmark

Abstract. Among the linear transformations of the span of annihilation and creation operators pertaining to a finite-dimensional space of single-fermion states, Bogolyubov transformations are those which preserve the anticommutator. Since this is a symmetric bilinear form, Bogolyubov transformations are orthogonal. A Bogolyubov transformation defines a quasi-fermion vacuum killed by the transformed annihilation operators. Applying the generator coordinate method to quasi-fermion vacua, including projecting a quasi-fermion vacuum onto the eigenspace of conserved quantum numbers, requires calculating the overlap amplitude between different vacua. Several different formulas for this amplitude in terms of the parameters of the generating Bogolyubov transformations carry in the literature the name of an "Onishi" formula, referring to a 1966 paper by Onishi and Yoshida. In particular the formula called so in the much cited book by Ring and Schuck differs from that of Onishi and Yoshida and has a wider scope. These formulas are often written with a square root and thus have a sign ambiguity. I show that this sign ambiguity stems from the fact that the representation of the orthogonal group of Bogolyubov transformations on the space of any number of fermions inhabiting the single-fermion state space is its spin representation, which is double valued. In the case of the general formula of Ring and Schuck, the sign ambiguity is therefore unavoidable. The formula of Onishi and Yoshida only applies when both vacua have non-zero overlap with the physical vacuum. They are then generated by a simply connected subset of the group. This renders their phases well defined, so the formula of Onishi and Yoshida has no sign ambiguity.

In 1983, Wüst and I devised a method to determine the unambiguous sign of the square root in the formula of Onishi and Yoshida. A different method was proposed by Robledo in 2009. I discuss the relation between these methods and show, in particular, how Robledo's formula follows directly from that of Onishi and Yoshida. Notably, neither Onishi and Yoshida nor their contemporary authors ever presented a derivation of their formula. Robledo based the derivation of his formula on Berezin integration. I discuss various ways to derive the formula of Onishi and Yoshida and various alternative ways to derive Robledo's formula.

1 Introduction

The term "Onishi" formula, introduced in [1], refers to a family of related formulas for the overlap amplitude of two Bogolyubov quasi-nucleon (more generally quasi-fermion) vacua. As a common feature, these formulas display a square root, which gives rise to an apparent sign ambiguity, first discussed by Wüst and me [2] and referred to in the literature as "the sign problem of the Onishi formula" or the like [3–12]. It is shown below that for some members of the family, this sign ambiguity is real and unavoidable while in some other cases it is not. The basis for my analysis is the observation that the group of Bogolyubov transformations pertaining to a given single-fermion state space is isomorphic to an orthogonal group and the representation of this group on the Fock space, the space of states of any number of fermions from the single-fermion state space, is just its so-called spin representation, described by Brauer and Weyl in 1935 [13]. It is the fundamental double-valuedness of the spin representation that gives rise to the sign ambiguity of some Onishi formulas.

I explain in Section 2 the said isomorphism between a group of Bogolyubov transformations and an orthogonal group. I then introduce the spin representation and explain its double-valuedness. I also introduce a coordinate representation, which displays in matrix form the action of the Bogolyubov transformation on annihilation and creation operators. It is pointed out that the double-valuedness of the spin representation gives rise to a fundamental sign ambiguity in the representation of Bogolyubov transformations by operators on the Fock space. Infinitesimal Bogolyubov transformations are discussed and properties of their coordinate and spin representations presented, leading to an explicit expression for the spin representation image of an arbitrary Bogolyubov transformation in the physically important case when the equivalent orthogonal transformation is unitary and proper.

Quasi-fermion vacua are introduced in Section 3 and it is explained that the sign ambiguity of the Fock space representation translates to fundamental sign ambiguity in the assignment of a quasi-fermion vacuum to a given Bogolyubov transformation. I then consider overlap amplitudes between different quasi-fermion vacua. Restricting my scope to the case of unitary and proper Bogolyubov transformations and even-dimensional single-fermion state spaces and using the expression for the Fock space representations of such Bogolyubov transformations obtained in Section 2, I derive the formula for the overlap amplitude that is called the "Onishi" formula in [1] under more general assumptions than made there.

The formula referred to by this name and presented originally by Onishi and Yoshida [14] is different. At the cost of a more limited scope it has *no* sign ambiguity. This is explained in Section 4. Variants of the formula of Onishi and Yoshida are discussed. Analysing the formula is shown, in particular, to lead to a general theorem on the characteristic roots of a product of two skew symmetric matrices which follows more directly from the properties of the Pfaffian of a skew symmetric matrix. As discussed in Section 5, this provides a direct link between the original formula of Onishi and Yoshida and a variant in terms of the Pfaffian presented by Robledo in 2009. The present paper is summarised in Section 6.

2 Bogolyubov Transformations are Orthogonal

Consider a space of single-fermion states of finite dimension d with orthonormal basic states $|i\rangle$ and corresponding annihilation operators a_i and creation operators $a_i^\dagger$. These operators span the space $\mathcal{F}$ of *field operators* $\alpha, \beta, \dots$ and generate the Clifford algebra $\mathrm{Cl}(2d)$. A *Bogolyubov transformation* g is a linear transformation of $\mathcal{F}$ that preserves the anticommutator $\{\alpha, \beta\}$. Since this is a non-degenerate, symmetric bilinear form, the group of Bogolyubov transformations can be identified with the group $\mathrm{O}(2d)$ of orthogonal transformations in $2d$ complex dimensions. The (faithful) *coordinate representation* $g \mapsto G$ of $\mathrm{O}(2d)$, where G is a $2d \times 2d$ matrix, is defined by $g\alpha_- = \alpha_- G$, where α_- denotes a row of basic field operators. A column of such operators is denoted by $\alpha_|$. Usually a Bogolyubov transformation is assumed to be also *unitary*. It then preserves also the Hermitian inner product $\{\alpha^\dagger, \beta\}$. The group of unitary Bogolyubov transformations form the subgroup $\mathrm{O}(2d, \mathbb{R})$ of orthogonal transformations in $2d$ real dimensions. One can distinguish finally between *proper* Bogolyubov transformations g with $\det g = 1$ and *improper* Bogolyubov transformations g with $\det g = -1$. The proper Bogolyubov transformations form subgroups $\mathrm{SO}(2d)$ and $\mathrm{SO}(2d, \mathbb{R})$ of $\mathrm{O}(2d)$ and $\mathrm{O}(2d, \mathbb{R})$, respectively. In the Fock space representation to be discussed below, the improper Bogolyubov transformations change the number parity.

Brauer and Weyl showed that $\mathrm{O}(2d)$ has a *double-valued* representation $g \mapsto \overline{g}$ in $\mathrm{Cl}(2d)$ [13], known as its *spin representation*. That the representation is double-valued means that $g_1 g_2 \mapsto \pm \overline{g}_1 \overline{g}_2$ and *a continuous path in* $\mathrm{O}(2d)$ *(indeed in* $\mathrm{SO}(2d, \mathbb{R})$*) from the identity* 1 *back to itself takes the representation image from* 1 *to* -1. The representation image $\overline{g}$ is defined by (i) $(g\alpha)\overline{g} = \overline{g}\alpha$ and (ii) $(\tau\overline{g})\overline{g} = 1$, where the operator τ inverts the factor order in a product of field operators. Here (i) determines $\overline{g}$ up to a numeric factor and (ii) fixes this factor within a sign. In consequence of the double-valuedness of the spin representation it is *impossible to map the entire group of Bogolyubov transformations continuously and single-valuedly into* $\mathrm{Cl}(2d)$ *in such a way that this map* $g \mapsto \overline{g}$ *obeys* (i) *for every* g *and* α. Indeed, even relaxing the normalisation condition (ii) by the multiplication of $\overline{g}$ by a continuous numeric factor cannot remove the double-valuedness. This holds upon restriction to $\mathrm{O}(2d, \mathbb{R})$, $\mathrm{SO}(2d)$ or $\mathrm{SO}(2d, \mathbb{R})$ and will be seen to be the origin of the sign ambiguity mentioned in the introduction.

Infinitesimal Bogolyubov transformations x obey $\{x\alpha, \beta\} + \{\alpha, x\beta\} = 0$ and form the Lie algebra $\mathfrak{o}(2d)$. In the basis of Hermitian field operators $a_i + a_i^\dagger$ and $-i(a_i - a_i^\dagger)$, the coordinate representation image of x is a skew symmetric matrix X. Its spin representation image $\overline{x}$ is $\frac{1}{2}\alpha_- X \alpha_|$. In the more usual basis $a_1, \dots, a_d, a_1^\dagger, \dots, a_d^\dagger$, one gets

$$X \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} X^T, \quad \overline{x} = \tfrac{1}{2}\alpha_- X \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \alpha_| \tag{1}$$

in terms of matrices with $d \times d$ blocks. (Details in [15].)

In most applications in nuclear physics, $g \in \mathrm{SO}(2d, \mathbb{R})$, that is, g is *unitary* and *proper*. Then in the basis of Hermitian field operators, G is real orthogonal and thus real-orthogonal equivalent to a block diagonal matrix with diagonal blocks

$$\begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} = \exp \begin{pmatrix} 0 & \phi \\ -\phi & 0 \end{pmatrix} \tag{2}$$

with real ϕ. Hence $G = \exp X$, where X is skew symmetric. Then X represents an infinitesimal Bogolyubov transformation x, and $g = \exp x$. In the basis of annihilation and creation operators, one gets from (1) that [2]

$$\overline{g} = \exp \overline{x} = \exp \tfrac{1}{2} \alpha_- X \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \alpha_| . \tag{3}$$

The angles ϕ are determined by G only modulo 2π and adding 2π to a single ϕ gives rise in (3) exactly to a change of sign of $\overline{g}$. This demonstrates the double-valuedness explicitly.

3 Quasi-Fermion Vacua and Their Overlaps

The field operators act on the space $\mathcal{K}$ of states of any number of fermions from the single-fermion state space. Formally, $\mathcal{K} = \mathrm{Cl}(2d)|\rangle$, where $|\rangle$ is a *vacuum state* characterised by $a_i|\rangle = 0$ for every i. In the terminology of Brauer and Weyl, it is the *spinor space* associated with $\mathrm{Cl}(2d)$. Given a Bogolyubov transformation g, a *quasi-fermion vacuum* $|g\rangle = 0$ obeys $g a_i |g\rangle = 0$ for every i. Part (i) of the definition of the spin representation implies $|g\rangle \propto \overline{g}|\rangle$, so the double-valuedness of the spin representation makes it *impossible to map the entire group of Bogolyubov transformations continuously and single-valuedly into* $\mathcal{K}$ *in such a way that this map* $g \mapsto |g\rangle$ *obeys* $g a_i |g\rangle = 0$ *for every* g *and* i. It is convenient to set $\langle|\rangle = 1$ and $|g\rangle = \pm\overline{g}|\rangle$. Then $\langle g|g\rangle = 1$ when g is unitary, and $|g_1 g_2\rangle = \pm\overline{g}_1|g_2\rangle$.

Structure calculations such as the projection of quasi-fermion vacua onto the state space of some conserved quantum numbers requires the calculation of overlap amplitudes $\langle g_1|g_2\rangle$. I assume from now on that g_1 and g_2 are unitary, which case covers the applications in nuclear physics. Then by $\langle g_1|g_2\rangle = \pm\langle|\overline{g}_1^\dagger \overline{g}_2|\rangle = \pm\langle|\overline{g}_1^{-1}\overline{g}_2|\rangle = \pm\langle|\overline{g_1^{-1} g_2}|\rangle$, an expression for $\langle|\overline{g}|\rangle$ for arbitrary g suffices for the calculation up to a sign of every $\langle g_1|g_2\rangle$. It can be shown that for improper g, the spin representation image $\overline{g}$ changes the number parity [15]. Since the vacuum has even number parity, $\langle|\overline{g}|\rangle = 0$ in this case. I can therefore assume further that g is proper, that is, $g \in \mathrm{SO}(2d, \mathbb{R})$. If also d is even, as usual in nuclear structure applications, one can then apply the Block-Messiah decomposition [16]

$$G = \begin{pmatrix} D^* & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} U & V \\ V & U \end{pmatrix} \begin{pmatrix} C^* & 0 \\ 0 & C \end{pmatrix} \tag{4}$$

to the coordinate representation image G in the basis of annihilation and creation operators. Here C and D are unitary and U and V are block diagonal with diagonal blocks

$$\begin{pmatrix} u & 0 \\ 0 & u \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & v \\ -v & 0 \end{pmatrix}, \tag{5}$$

where $u, v \geq 0$ and $u^2 + v^2 = 1$. Since each factor in (4) is the coordinate representation image of some $g \in \mathrm{SO}(2d, \mathbb{R})$, the Block-Messiah decomposition corresponds to a decomposition $g = g_D g_W g_C$ with $g_D, g_W, g_C \in \mathrm{SO}(2d, \mathbb{R})$.

The contribution to $\langle|\overline{g}|\rangle$ of each factor g_D, g_W and g_C can be evaluated by means of (3). The result is $\langle| \, \overline{g}_D = \sqrt{|D^*|} \, \langle|$ and $\overline{g}_C \, |\rangle = |\rangle \, \sqrt{|C^*|}$ with indefinite signs due to the multi-valuedness of each X as a function of the corresponding G, and $\langle|\overline{g}_W|\rangle = \prod u = \sqrt{|U|} \geq 0$ [15]. When G is expressed in the form

$$G = \begin{pmatrix} A^* & B \\ B^* & A \end{pmatrix}, \tag{6}$$

this combines to $\langle|\overline{g}|\rangle = \sqrt{|D^* U C^*|} = \sqrt{|A^*|}$ with an indefinite sign of the square root as anticipated from the indefinite sign of $\overline{g}$. In the present derivation, the indefiniteness is seen to be due to indefinite signs of $\sqrt{|D^*|}$ and $\sqrt{|C^*|}$, while $\sqrt{|U|} \geq 0$. The equivalent result $\langle g|\rangle = \sqrt{|A|}$ is derived in [1] in the case $D = C = 1$, which can be generalised to the case when A is Hermitian and positive semi-semidefinite ($D = C^\dagger$). In that case, $|A^*| = |A| \geq 0$. The expression $\langle g|\rangle = \sqrt{|A|}$ is called the "Onishi" formula in [1].

4 Formula of Onishi and Yoshida

The name of an "Onishi" formula refers to a 1966 paper by Onishi and Yoshida [14]. These authors consider, however, not the normalised state $|g\rangle$, but the unnormalised state

$$|\tilde{g}\rangle = \frac{|g\rangle}{\langle|g\rangle} = \exp \tfrac{1}{2} a_{-}^\dagger F a_{|}^\dagger \, |\rangle, \tag{7}$$

where $F = (BA^{-1})^* = -F^T$. The last expression in (7) is the Thouless expansion [17]. Note that $|\tilde{g}\rangle$ has *no phase ambiguity*. Its normalisation is fixed by $\langle|\tilde{g}\rangle = 1$. This comes at the cost that it is defined only when $\langle|g\rangle \neq 0$ or, equivalently, $|A| \neq 0$. Onishi and Yoshida write

$$\langle \tilde{g}_1 | \tilde{g}_2 \rangle = \exp \tfrac{1}{2} \mathrm{tr} \, \log(1 + F_1^\dagger F_2). \tag{8}$$

Notably, a *derivation* of this expression is given by neither Onishi and Yoshida nor their contemporary authors [18–20], all of whom refer to [14]. A fairly short derivation is shown in [15], and other derivations were also presented more recently [10, 12].

Note that $\exp \frac{1}{2} a_-^\dagger F a_|^\dagger$ is a *polynomial* in the entries of F because at most d creation operators can be multiplied together to a non-zero result. Therefore in

$$\langle \tilde{g}_1 | \tilde{g}_2(z) \rangle = \exp \tfrac{1}{2} \mathrm{tr} \log(1 + z F_1^\dagger F_2) = \sqrt{|1 + z F_1^\dagger F_2|}, \tag{9}$$

where $\tilde{g}(z) = \exp \frac{1}{2} a_-^\dagger z F a_|^\dagger |\rangle$, the first expression, and therefore also the second and the third, are polynomials in z provided in the latter two, we take $\log 1 = 0$ and $\sqrt{1} = 1$ and require continuity in z. It follows in particular that then both the latter are well defined for every z. The last expression in (9) is a polynomial in z only if the non-zero characteristic roots of $F_1^\dagger F_2$ have even multiplicities, so we can write, in fact,

$$\langle \tilde{g}_1 | \tilde{g}_2 \rangle = \prod{}' (1 + r), \tag{10}$$

where the product runs over one out of each pair of equal characteristic roots r of $F_1^\dagger F_2$ [2].

The only assumption was that $F_1^\dagger$ and F_2 be skew symmetric, so it was proved, in fact, that *whenever two square matrices P and Q of equal dimensions are skew symmetric, the characteristic roots of their product PQ have even multiplicities.* This follows much more directly from the following result due to Cayley: *When P is skew symmetric, $|P| = (\mathrm{pf}\, P)^2$, where* pf P *is a polynomial in the entries of P* (called its *Pfaffian*) [21]. One calculates, in fact,

$$|1 + zPQ| = \begin{vmatrix} 1 + zPQ & -zP \\ 0 & 1 \end{vmatrix} = \begin{vmatrix} zP & 1 \\ -1 & Q \end{vmatrix} \begin{vmatrix} Q & -1 \\ 1 & 0 \end{vmatrix} = \begin{vmatrix} zP & 1 \\ -1 & Q \end{vmatrix} = \left(\mathrm{pf} \begin{pmatrix} zP & 1 \\ -1 & Q \end{pmatrix} \right)^2, \tag{11}$$

whence the assertion follows [15]. A more elaborate proof under certain restricting assumptions is found in [22].

5 Robledo Formula

A standard expression for the Pfaffian [21] gives

$$\mathrm{pf} \begin{pmatrix} 0 & 1 \\ -1 & Q \end{pmatrix} = (-1)^{d(d-1)/2}. \tag{12}$$

Setting $\sqrt{1} = 1$ and assuming continuity in z, one can therefore write (11) in the form

$$\sqrt{|1 + zPQ|} = (-)^{d(d-1)/2}\, \mathrm{pf} \begin{pmatrix} zP & 1 \\ -1 & Q \end{pmatrix}, \tag{13}$$

so that for $z = 1$, the expression (9) becomes

$$\langle \tilde{g}_1 | \tilde{g}_2 \rangle = (-)^{d(d-1)/2}\, \mathrm{pf} \begin{pmatrix} F_1^\dagger & 1 \\ -1 & F_2 \end{pmatrix}. \tag{14}$$

In 2009, Robledo got this expression by Berezin integration [23] in a slightly different but equivalent form [6]. Other derivations have appeared more recently [10, 12], and yet another, combinatoric, one is presented in [15].

6 Summary

The group of Bogolyubov transformation pertaining to a given finite-dimensional single-fermion state space was explained to be isomorphic to an orthogonal group and its representation on the Fock space, which is the space of states of any number of fermions from the single-fermion state space, to be just the spin representation of this group. The double-valuedness of the spin representation was shown to lead to a fundamental sign ambiguity in the assignment of an operator on the Fock space to a given Bogolyubov transformation, which translates to a corresponding sign ambiguity in the assignment of a quasi-fermion vacuum to such a transformation and also to a sign ambiguity in the formula for the overlap amplitude of two quasi-fermion vacua that is called the "Onishi" formula in the much cited book by Ring and Schuck [1]. On the other hand the original formula of Onishi and Yoshida which is referred to by this name has no sign ambiguity. This comes at the cost of a more limited scope. Versions of this formula were discussed. Analysing it leads to a general theorem on the characteristic roots of the product of two skew symmetric matrices which follows more directly from the properties of the Pfaffian of a skew symmetric matrix. This provides a direct link between the original formula of Onishi and Yoshida and a variant in terms of the Pfaffian presented by Robledo in 2009.

References

[1] P. Ring, P. Schuck, *The Nuclear Many-Body Problem*, Springer-Verlag, Berlin (1980).
[2] K. Neergård, E. Wüst, *Nucl. Phys. A* **402** (1983) 311.
[3] K.W. Schmid, *Prog. Part. Nucl. Phys.* **52** (2004) 565.
[4] M. Oi, N. Tajima, *Phys. Lett. B* **606** (2005) 43.
[5] M. Bender, P.-H. Heenen, *Phys. Rev. C* **78** (2008) 024309.
[6] L.M. Robledo, *Phys. Rev. C* **79** (2009) 021302.
[7] B. Avez, M. Bender, *Phys. Rev. C* **85** (2012) 034325.
[8] G.F. Bertsch, L.M. Robledo, *Phys. Rev. Lett.* **108** (2012) 042505.
[9] T. Mizusaki, M. Oi, *Phys. Lett. B* **715** (2012) 219.
[10] T. Mizusaki, M. Oi, N. Shimizu, *Phys. Lett. B* **779** (2018) 237.
[11] B. Bally, T. Duguet, *Phys. Rev. C* **97** (2018) 024304.
[12] A. Porro, T. Duguet, *Eur. J. Phys. A* **58** (2022) 197.
[13] R. Brauer, H. Weyl, *Am. J. Math.* **57** (1935) 425.
[14] N. Onishi, S. Yoshida, *Nucl. Phys. A* **80** (1966) 367.
[15] K. Neergård, *Phys. Rev. C* **107** (2023) 0243158.
[16] C. Bloch, A. Messiah, *Nucl. Phys.* **39** (1962) 95.

[17] D.J. Thouless, *Nucl. Phys.* **21** (1960) 225.
[18] R. Beck, H.J. Mang, P. Ring, *Z. Phys.* **231** (1970) 26.
[19] K. Goeke, A. Faessler, H.H. Wolter, *Nucl. Phys. A* **183** (1972) 352.
[20] K. Goeke, J. Garcia, A. Faessler, *Nucl. Phys. A* **208** (1973) 477.
[21] A. Cayley, *J. reine angew. Math.* **38** (1849) 93.
[22] M. Oi, T. Mizusaki, N. Shimizu, Y. Sun, *EPJ Web of Conf.* **223** (2019) 01047.
[23] F.A. Berezin, *The Method of Second Quantization*, Academic Press, New York (1966).