Fock space representations of Bogolyubov transformations as spin representations

K. Neergård
Fjordtoften 17, 4700 Næstved, Denmark

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The representation on a Fock space of the group of Bogolyubov transformations is recognized as the spin representation of an orthogonal group. Derivations based on this observation of some known formulas for the overlap amplitude of two Bogolyubov quasifermion vacuum states that are in some cases more complete than those in the literature are shown. It is pointed out that the name of an "Onishi formula" is assigned in the literature to two different expressions which are related but have different scopes. One of them has what has been described as a sign problem; the other one, due to Onishi and Yoshida, has a more limited scope and no sign problem. I give a short proof of the latter, whose derivation is missing in the paper by Onishi and Yoshida, and a new, combinatoric, proof of an equivalent formula recently derived by Robledo.

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I. INTRODUCTION

Bogolyubov quasinucleon vacua and their overlap amplitudes are ubiquitous in contemporary calculations of nuclear structure. For a review, see [1]. Methods such as the generator coordinate method [2] and, more specifically, the projection of a quasinucleon vacuum onto the state space of some conserved quantum numbers [3] require the calculation of overlap amplitudes between different vacua. Some formulas for such overlap amplitudes involve a square root. This gives rise to a sign ambiguity that has been called in the literature "the sign problem of the Onishi formula" or similar [4–13], referring to a paper by Onishi and Yoshida [14]. This sign ambiguity was first discussed by Wüst and me after being recognized in the context of quantum number projection of cranked quasinucleon vacua [15]. [Our paper has an unfortunate error. From (3.4) onwards, every matrix transposition except the second one in the first line on page 321 should be a Hermitian conjugation.] The ambiguity is shown in the present paper to be related to the well known double-valuedness of the representation of spatial rotations on the spin states of a spin $1/2$ fermion, which is the simplest in a family of double-valued, so-called spin representations of orthogonal transformations.

A Bogolyubov quasinucleon vacuum, or, more generally, quasifermion vacuum, is determined by the Bogolyubov transformation that relates its annihilation operators to those of the physical vacuum or some other reference vacuum. In Sec. II, I first recall the known fact that the group of Bogolyubov transformations related to some finite-dimensional space of single-fermion states is isomorphic to an orthogonal group, and then briefly review the theory of spin representations. The relation to physics is established by the observation that the Fock space, that is, the space of states of any number of fermions inhabiting the space of single-fermion states, has the structure of a spinor space and therefore carries a spin representation of the group. In most applications, Bogolyubov transformations are assumed to be unitary with unit determinant. At the end of Sec. II, I give the details of a derivation of an expression for the spin-representation image of such a Bogolyubov transformation that appears in [15] without a proof.

This expression forms the basis for a derivation in Sec. III of a formula for the overlap amplitude of two arbitrary members of a large class of quasifermion vacua in terms of their generating Bogolyubov transformations, that is called the "Onishi formula" in the much cited book by Ring and Schuck [16]. My derivation does not require certain restricting assumptions made there and in some earlier work. I also rederive some formulas in the literature for the matrix element between two Bogolyubov vacua of the transformation of the Fock space generated by a unitary transformation of the single-fermion state space, and show that all these formulas have an unavoidable sign ambiguity due to the double-valuedness of the spin representation.

The "Onishi formula" of Ring and Schuck is not the formula of Onishi and Yoshida. Their formula for the overlap amplitude of two quasifermion vacua has a more limited scope as it applies only when these vacua have nonzero overlaps with the reference vacuum. Due to this restriction, it has no sign ambiguity. Notably, Onishi and Yoshida do not show a derivation of their formula. I give in Sec. IV a short proof of it by repeated application of a relation mentioned in their paper.

Wüst and I devise in [15] a method to calculate numerically the unambiguous overlap amplitude of Onishi and Yoshida. Recently, Robledo proposed another method which may be numerically more stable [7]. I show in Sec. V that Robledo's formula can be derived directly from that of Onishi and Yoshida. Robledo's derivation is based on Berezin integration, and recently some other derivations appeared [11,13]. Before summarizing the paper in Sec. VI, I show at the end of Sec. V yet another, combinatoric, derivation.

II. FOCK SPACE REPRESENTATION OF THE BOGOLYUBOV GROUP

Most structure calculations in atomic, molecular, and nuclear physics employ a space $\mathcal{S}$ of single-fermion states of finite dimension d. Corresponding to orthonormal basic states $|i\rangle$ in $\mathcal{S}$ one can define annihilation operators a_i. I call *field operators* the linear combinations α of a_i and $a_i^\dagger$ and denote by $\mathcal{F}$ the $2d$-dimensional space of these operators. A *Bogolyubov transformation* [17] is a linear transformation of $\mathcal{F}$ that preserves the anticommutator $\{\alpha, \beta\}$. Since the anticommutator is a symmetric bilinear form, the group of Bogolyubov transformations, which I call the *Bogolyubov group*, is isomorphic to the group $\mathrm{O}(2d)$ of orthogonal transformations in $2d$ complex dimensions, and I identify the Bogolyubov group with $\mathrm{O}(2d)$. Given any basis for $\mathcal{F}$, I denote by α_- and $\alpha_|$ the row and column of the basic field operators. The *coordinate representation* $g \mapsto G$ of $\mathrm{O}(2d)$ in this basis is then defined by $g\alpha_- = \alpha_- G$, so that $g_1 g_2 \mapsto G_1 G_2$, where G is a $2d \times 2d$ matrix. This is a faithful representation; that is, G determines g.

Usually a Bogolyubov transformation is assumed to be also *unitary* in the sense that it preserves the Hermitian inner product $\{\alpha^\dagger, \beta\}$ in $\mathcal{F}$. See, however, [18] for an exception. The Hermitian field operators $\alpha_{i+} = a_i + a_i^\dagger$ and $\alpha_{i-} = -i(a_i - a_i^\dagger)$ obey $\{\alpha_{is}, \alpha_{i's'}\} = \{\alpha_{is}^\dagger, \alpha_{i's'}\} = 2\delta_{is,i's'}$. (The use of i both as an index and to denote the imaginary unit should cause no confusion.) In this basis, the condition of simultaneous orthogonality and unitarity reads $G^T G = G^\dagger G = 1$, where 1 denotes the unit matrix. Hence G is real. This implies, in particular, that $g\alpha^\dagger = (g\alpha)^\dagger$. The group of unitary Bogolyubov transformations, the *unitary Bogolyubov group*, is thus isomorphic to the group $\mathrm{O}(2d, \mathbb{R})$ of orthogonal transformations in $2d$ real dimensions associated with a positive definite quadratic form, and I identify the unitary Bogolyubov group with $\mathrm{O}(2d, \mathbb{R})$. This isomorphism of the unitary subgroup of a complex orthogonal group to the real subgroup was pointed out by Weyl [19], and the isomorphism of the general and unitary Bogolyubov groups to the complex and real orthogonal groups in $2d$ dimensions was noticed by Balian and Brezin [18]. Most of the discussion of $\mathrm{O}(2d)$ in the present section applies almost verbatim also to $\mathrm{O}(2d, \mathbb{R})$. I shall in general not mention explicitly the modifications pertaining to this case.

The group $\mathrm{O}(2d)$ has a maximal connected subgroup $\mathrm{SO}(2d)$ of index 2. The transformations in $\mathrm{SO}(2d)$ have determinant 1 and those in its, also connected, coset determinant -1 [19]. That these sets are connected means that there is a continuous path between any two elements. The elements of $\mathrm{SO}(2d)$ may be seen as rotations of the $2d$-dimensional space and those of the coset as combinations of a rotation and a reflection. These two types of orthogonal transformations are sometimes called proper and improper, and one can distinguish accordingly between proper and improper Bogolyubov transformations.

The *Fock space* $\mathcal{K}$ associated with $\mathcal{S}$ is the space of states formed by the action of a polynomial in the creation operators $a_i^\dagger$ on a state killed by the annihilation operators a_i and conceived as a vacuum state. It has the structure of a *spinor space* [20]. The operators on $\mathcal{K}$ form an algebra isomorphic to the Clifford algebra [21] $\mathrm{Cl}(2d)$, and I identify the algebra of operators on $\mathcal{K}$ with $\mathrm{Cl}(2d)$. Every element of $\mathrm{Cl}(2d)$ can then be written as a a polynomial in field operators. It was shown by Brauer and Weyl that $\mathrm{O}(2d)$ has a *double-valued* representation on the spinor space $\mathcal{K}$, the so-called *spin representation* [20]. Specifically, this representation maps every $g \in \mathrm{O}(2d)$ to a *pair* $\pm\bar{g}$ of elements of $\mathrm{Cl}(2d)$ in such a way that $g_1 g_2 \mapsto \pm\bar{g}_1\bar{g}_2$, and there is a path in $\mathrm{SO}(2d)$ from the identity 1 back to itself which connects its images ± 1 continuously. As pointed out by Weyl [19], the second property implies that the connected sets, $\mathrm{SO}(2d)$ and its improper coset, are not *simply* connected: this path cannot be contracted to a point. That (unitary) Bogolyubov groups are not simply connected was noticed in [15].

The representation $g \mapsto \pm\bar{g}$ is defined in [20] by

$$(g\alpha)\bar{g} = \bar{g}\alpha \tag{1}$$

and

$$(\tau\bar{g})\bar{g} = 1, \tag{2}$$

where τ is the linear operator on $\mathrm{Cl}(2d)$ that inverts the order of the factors in every product of field operators. For a given g, the condition (1) determines $\bar{g}$ within a numeric factor, and the condition (2) fixes this factor up to a sign. Since both conditions are compatible with the group relations, they thus define a *possibly* double-valued *representation*. The fact that this representation turns out *actually* double-valued implies that *the entire Bogolyubov group (or its unitary subgroup) cannot be mapped continuously and single-valuedly into the space of linear transformations of the Fock space in such a way that this map $g \mapsto \bar{g}$ obeys (1) for every g and α. This will turn out in Sec. III to be the origin of the so-called sign problem of the Onishi formula mentioned in the Introduction.* In fact, (1) alone allows the normalized $\bar{g}$ to be multiplied by a g-dependent numeric factor, but for the resulting map to be continuous, this factor must depend continuously on g, so the resulting map remains double-valued. From now on, $\bar{g}$ is understood to satisfy both conditions (1) and (2).

The space $\mathrm{Cl}(2d)$ of operators on $\mathcal{K}$ is the direct sum of subspaces $\mathrm{Cl}_\pm(2d)$ formed by the operators that can be expressed by polynomials in field operators whose terms have only even and only odd degree, respectively. Evidently $\mathrm{Cl}_\pm(2d)\,\mathrm{Cl}_\pm(2d) = \mathrm{Cl}_+(2d)$ and $\mathrm{Cl}_+(2d)\,\mathrm{Cl}_-(2d) = \mathrm{Cl}_-(2d)\,\mathrm{Cl}_+(2d) = \mathrm{Cl}_-(2d)$. For the reflection g of $\mathcal{F}$ along the direction of the vector α_{1+}, that is,

$$\alpha_{1+} \mapsto -\alpha_{1+}, \quad \alpha_{is} \mapsto \alpha_{is} \text{ for } is \neq 1+, \tag{3}$$

the operator

$$\bar{g} = \prod_{is \neq 1+} \alpha_{is}, \tag{4}$$

obeys (1) and (2). The order of the factors in (4) is immaterial since reordering changes at most the sign of the product. Orthogonal transformation gives an analogous expression for a spin-representation image of any other reflection, and all these images belong to $\mathrm{Cl}_-(2d)$. Since every proper orthogonal transformation is the product of an even number of reflections, and every improper orthogonal transformation a product of an odd number of reflections [22], it follows that the spin representation maps $\mathrm{SO}(2d)$ into $\mathrm{Cl}_+(2d)$, and its improper coset into $\mathrm{Cl}_-(2d)$. This construction succeeds in $\mathrm{O}(2d, \mathbb{R})$. There, the spin-representation image of every reflection is unitary, whence it follows that the image of every g is unitary. The spin representation of $\mathrm{O}(2d)$ is irreducible but splits upon restriction to SO$(2d)$ into two inequivalent irreducible components carried by the subspaces $\mathcal{K}_\pm$ of $\mathcal{K}$ with even and odd particle numbers, respectively [20].

The *Lie algebra* of a continuous linear group is the anticommutative algebra (the *definition* of a Lie algebra) of infinitesimal deviations of group elements from the identity 1 with the commutator product [19]. I denote by $\mathfrak{o}(2d)$ the Lie algebra of O$(2d)$ and identify it with its realization on $\mathcal{F}$. The Lie algebra $\mathfrak{o}(2d)$ then consists of the linear transformations $\alpha \mapsto x\alpha$ of $\mathcal{F}$ that obey $\{x\alpha, \beta\} + \{\alpha, x\beta\} = 0$. In the basis of field operators α_{is}, the matrices X of its coordinate representation $x \mapsto X$ are skew symmetric. Upon restriction to $\mathfrak{o}(2d, \mathbb{R})$ they are also real. In the basis $a_1, \dots, a_d, a_1^\dagger, \dots, a_d^\dagger$, they obey

$$X\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} X^T, \tag{5}$$

in terms of block matrices with $d \times d$ blocks, and X is anti-Hermitian upon restriction to $\mathfrak{o}(2d, \mathbb{R})$. The spin representation of O$(2d)$ gives rise in the infinitesimal limit to two inequivalent irreducible (single-valued) spin representations of $\mathfrak{o}(2d)$ carried by the same subspaces of $\mathcal{K}$ as those of SO$(2d)$ [20]. These representations were discovered in their abstract forms by Cartan before the work of Brauer and Weyl [23].

Let x denote an element of $\mathfrak{o}(2d)$, let X be the corresponding matrix in the coordinate representation pertaining to some basis for $\mathcal{F}$, and let $\bar{x}$ be the spin representation image of x. Inserting $g = 1 + x$ in (1) and linearizing in x gives

$$x\alpha_- = \alpha_- X = [\bar{x}, \alpha_-]. \tag{6}$$

Since in a neighborhood of 1 the transformation g belongs to SO$(2d)$, the operator $\bar{x}$ belongs to Cl$_+(2d)$, and, in order that $[\bar{x}, \alpha_-]$ be linear in the field operators, it must then be given by a quadratic polynomial in field operators. In the basis $a_1, \dots, a_d, a_1^\dagger, \dots, a_d^\dagger$, the complete solution of the last equation in (6) is then

$$\bar{x} = \frac{1}{2}\alpha_- X \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \alpha_| + \gamma \tag{7}$$

with an arbitrary numeric constant γ. The normalization (2) gives $\gamma = 0$, so

$$\bar{x} = \frac{1}{2}\alpha_- X \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \alpha_|. \tag{8}$$

Note that the matrix sandwiched here between α_- and $\alpha_|$ is skew symmetric due to (5). Given the representation $x \mapsto \bar{x}$, one can determine $\bar{g}$ for $g \in$ SO$(2d)$ by integrating the differential equation $\bar{g}'(t) = \bar{x}(t)\bar{g}(t)$ along a path $g(t)$, $0 \leqslant t \leqslant 1$, such that $g(0) = 1$, $g(1) = g$, and $g'(t) = x(t)g(t)$. Choosing different paths gives the two solutions for $\bar{g}$ with opposite signs.

Now assume $g \in$ SO$(2d, \mathbb{R})$. I the basis of field operators α_{is}, the matrix G is then real orthogonal, and $|G| = 1$, so G is real-orthogonal equivalent to a block diagonal matrix with diagonal blocks of the form

$$\begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} = \exp\begin{pmatrix} 0 & \phi \\ -\phi & 0 \end{pmatrix}, \tag{9}$$

where ϕ is real. It follows that $G = \exp X$, where X is real and skew symmetric and thus represents an element x of $\mathfrak{o}(2d, \mathbb{R})$. The relation $G = \exp X$ translates to $g = \exp x$. Because $g(t) = \exp tx$, $0 \leqslant t \leqslant 1$, defines a path from 1 to g with $g'(t) = xg(t)$, this translates, in turn, to $\bar{g} = \exp \bar{x}$, where $\bar{g}$ is one of the two spin-representation images of g. In the basis $a_1, \dots, a_d, a_1^\dagger, \dots, a_d^\dagger$, the expression (8) gives

$$\bar{g} = \exp \frac{1}{2}\alpha_- X \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \alpha_|. \tag{10}$$

This is essentially (2.11) in [15], where X is written as $\log G$. The angles ϕ in (9) are not unique; the same G results when an arbitrary integral multiple of 2π is added to each ϕ. In (10), this gives rise, exactly, to the sign ambiguity of $\bar{g}$. In fact, when just one of the angles ϕ varies continuously from 0 to 2π while the rest are kept at 0, the transformation g goes from 1 back to itself, but $\bar{g}$ goes from 1 to -1. Since this path runs within O$(2d, \mathbb{R})$, the double-valuedness persists upon restriction to this subgroup [20].

Adding an integral multiple of 2π to each ϕ corresponds in the basis $a_1, \dots, a_d, a_1^\dagger, \dots, a_d^\dagger$ to adding an arbitrary integral multiple of $2\pi i$ to each eigenvalue of the anti-Hermitian matrix X. Bally and Duguet propose to choose for these eigenvalues always the principal logarithms of those of G [12]. This renders $\bar{g}$ discontinuous at the branch cuts of the logarithms, and the map $g \mapsto \bar{g}$ will not preserve the group relations.

III. QUASIFERMION VACUA AND THEIR OVERLAPS

In the structure calculations, one is specifically interested in the *quasifermion vacuum states* $|g\rangle$, which are states annihilated by the transformed annihilation operators ga_i. It follows from (1) that $|g\rangle \propto \bar{g}|\rangle$, where $|\rangle$ denotes a "reference" state annihilated by the field operators a_i. The latter need not be thought of as representing the physical vacuum. As pointed out by Bally and Duguet [12], every state proportional to some $\bar{g}|\rangle$ may serve as a reference state. This follows from the Bogolyubov transformations forming a group. When $|\rangle$ is fixed, the double-valuedness of the map $g \mapsto \bar{g}$ implies double-valuedness of the map $g \mapsto \bar{g}|\rangle$. An argument as in Sec. II shows that the double-valuedness persists if $\bar{g}|\rangle$ is multiplied by a g-dependent numeric factor, as done, for example, in the theory of Bally and Duguet. Therefore *the entire Bogolyubov group (or its unitary subgroup) cannot be mapped continuously and single-valuedly into the Fock space in such a way that this map $g \mapsto |g\rangle$ obeys $(ga_i)|g\rangle = 0$ for every g and i.* Since any g-dependent numeric factor is well defined in a given formalism, it is interesting to analyze the bare expression $|g\rangle = \pm\bar{g}|\rangle$, which implies $|g_1 g_2\rangle = \pm\bar{g}_1|g_2\rangle$. So from now on, this is the definition of $|g\rangle$.

As noted in the Introduction, overlap amplitudes $\langle g_1|g_2\rangle$ are central in many types of calculations. I limit my discussion of such amplitudes to *unitary* Bogolyubov transformations. Then every $\bar{g}$ is unitary, whence follows $\bar{g}^{-1} = \bar{g}^{-1} = \bar{g}^\dagger$. I also assume $\langle|\rangle = 1$, which then implies $\langle g|g\rangle = 1$ for every

g. The relation $\langle g_1|g_2\rangle = \langle|\bar{g}_1^\dagger \bar{g}_2|\rangle = \langle|\bar{g}_1^{-1}\bar{g}_2|\rangle = \langle|\overline{g_1^{-1}g_2}|\rangle$ reduces the calculation of $\langle g_1|g_2\rangle$ to the calculation of some $\langle|\bar{g}|\rangle$ [16]. One can assume $g \in \mathrm{SO}(2d,\mathbb{R})$ because otherwise $\bar{g} \in \mathrm{Cl}_-(2d)$, whose elements connect the subspaces $\mathcal{K}_\pm$ of $\mathcal{K}$, whence $\langle|\bar{g}|\rangle = 0$ because $|\rangle \in \mathcal{K}_+$. When also *$d$ is even*, as usual in nuclear structure calculations, a formula for $\langle|\bar{g}|\rangle$ can then be derived from the Bloch-Messiah decomposition [24] of the matrix G representing g in the coordinate representation pertaining to the basis $a_1,\dots,a_d,a_1^\dagger,\dots,a_d^\dagger$. In the notation of Beck, Mang, and Ring [25], this decomposition reads

$$G = \begin{pmatrix} D^* & 0 \\ 0 & D \end{pmatrix}\begin{pmatrix} U & V \\ V & U \end{pmatrix}\begin{pmatrix} C^* & 0 \\ 0 & C \end{pmatrix}, \tag{11}$$

where D and C are unitary and U and V are block diagonal with 2×2 diagonal blocks

$$\begin{pmatrix} u & 0 \\ 0 & u \end{pmatrix} \quad\text{and}\quad \begin{pmatrix} 0 & v \\ -v & 0 \end{pmatrix}. \tag{12}$$

Here, u and v are non-negative and obey $u^2+v^2=1$. Each of the three factors Γ in (11) is unitary and has unit determinant. Further, each of them obeys the condition of orthogonality

$$\Gamma\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\Gamma^T = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{13}$$

which for a unitary Γ is equivalent to

$$\Gamma\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\Gamma^*. \tag{14}$$

Thus each of them represents a proper unitary Bogolyubov transformation, which I denote by g_D, g_W, and g_C, respectively. I set out to analyze the action of each of these three factors of the product $g = g_D g_W g_C$.

To calculate the action of g_C, let the basic single-fermion states $|i\rangle$ be chosen such that C is diagonal. Since C is unitary, one can set $C = \exp Y$, where Y is diagonal and imaginary. I denote by y_i the diagonal entries in Y. The rightmost matrix in (11) becomes $\exp X$, where X is block diagonal with $-Y$ in the upper diagonal block and Y in the lower diagonal block. Then (8) gives

$$\bar{x} = \frac{1}{2}\sum_i y_i(a_i^\dagger a_i - a_i a_i^\dagger) = \sum_i y_i\left(a_i^\dagger a_i - \frac{1}{2}\right), \tag{15}$$

whence

$$\bar{g}_C\,|\rangle = \exp\bar{x}\,|\rangle = \exp\left(-\frac{1}{2}\sum y_i\right)|\rangle = \sqrt{|C^*|}\,|\rangle. \tag{16}$$

Analogously, $\langle|\,\bar{g}_D = \sqrt{|D^*|}\,\langle|$.

One can set

$$\begin{pmatrix} U & V \\ V & U \end{pmatrix} = \exp X, \tag{17}$$

where

$$X = \begin{pmatrix} 0 & Y \\ Y & 0 \end{pmatrix}, \tag{18}$$

and Y is block diagonal with 2×2 diagonal blocks

$$\begin{pmatrix} 0 & y \\ -y & 0 \end{pmatrix} \tag{19}$$

such that $\cos y = u$ and $\sin y = v$. With y_i denoting the entry of Y with indices $i, i+1$, where i is odd, one gets from (8) that

$$\bar{x} = \sum_{\text{odd } i} y_i(a_i a_{i+1} + a_i^\dagger a_{i+1}^\dagger). \tag{20}$$

By

$$\begin{aligned}(a_i a_{i+1} &+ a_i^\dagger a_{i+1}^\dagger)^2|\rangle \\ &= (a_i a_{i+1} a_i^\dagger a_{i+1}^\dagger + a_i^\dagger a_{i+1}^\dagger a_i a_{i+1})|\rangle = -|\rangle\end{aligned} \tag{21}$$

it follows that

$$\langle|\bar{g}_W|\rangle = \langle|\exp\bar{x}|\rangle = \prod_{\text{odd } i}\cos y_i = \prod_{\text{odd } i} u_i = \sqrt{|U|}, \tag{22}$$

where u_i are the diagonal entries of U, and the non-negative square root is taken in the last expression.

Combining these results gives

$$\langle|\bar{g}|\rangle = \sqrt{|D^*UC^*|} = \sqrt{|A^*|} \tag{23}$$

in the notation of [25], where

$$G = \begin{pmatrix} A^* & B \\ B^* & A \end{pmatrix}. \tag{24}$$

The appearance of a square root in (23) reflects the sign ambiguity of $\bar{g}$. In the derivation above, it stems from the multivaluedness of Y as a solution of $C = \exp Y$ or $D = \exp Y$. In [16], the identity $\langle g|\rangle = \sqrt{|A|}$, which is equivalent to (23), is derived in the case $D = C = 1$, which may be generalized by a change of basis for $\mathcal{S}$ to the case when A is Hermitian and positive semidefinite. In that case, $|A^*| = |A| \geqslant 0$.

From (23) and (24), one gets immediately

$$\langle g_1|g_2\rangle = \langle|\bar{g}_1^{-1}\bar{g}_2|\rangle = \sqrt{|A_1^T A_2^* + B_1^T B_2^*|} = \sqrt{|A_2^\dagger A_1 + B_2^\dagger B_1|}. \tag{25}$$

The last expression is (2.14a) in [25], where it is derived from (32) with a specific choice of D_1, C_1, D_2, and C_2. In [16], it is derived from $\langle g|\rangle = \sqrt{|A|}$.

In quantum number projection, one needs matrix elements $\langle g_1|\bar{u}|g_2\rangle$, where $\bar{u}$ is the unitary transformation of $\mathcal{K}$ generated by a unitary transformation u of $\mathcal{S}$. Explicitly, $\bar{u} = \exp a_-^\dagger\, Y\, a_|$, where $u = \exp y$ and $y|i\rangle_- = |i\rangle_- Y$ with $|i\rangle_-$ denoting the row of states $|i\rangle$, and $a_-^\dagger$ is the row of operators $a_i^\dagger$, and $a_|$ the column of operators a_i. The operator

$$a_-^\dagger\, Y\, a_| = \frac{1}{2}\left[\alpha_-\begin{pmatrix} 0 & -Y^T \\ Y & 0 \end{pmatrix}\alpha_| + \operatorname{tr} Y\right] \tag{26}$$

with α_- and $\alpha_|$ as in (8) is, except for the last term in the brackets, the spin representation image $\bar{x}$ of the element x of $\mathfrak{o}(2d,\mathbb{R})$ with

$$X = \begin{pmatrix} -Y^T & 0 \\ 0 & Y \end{pmatrix} = \begin{pmatrix} Y^* & 0 \\ 0 & Y \end{pmatrix}, \tag{27}$$

where the last transformation stems from X being anti-Hermitian. Therefore $\bar{u}\exp -\frac{1}{2}\operatorname{tr} Y = \bar{u}/\sqrt{|U|}$, with $U = \exp Y$, is the spin representation image of the element g of

$SO(2d, \mathbb{R})$ determined by

$$G = \begin{pmatrix} U^* & 0 \\ 0 & U \end{pmatrix}. \tag{28}$$

Using $|U| = |U^T|$, one arrives at

$$\begin{aligned}\langle g_1|\bar{u}|g_2\rangle &= \langle|\bar{g}_1^{-1}\bar{g}\,\bar{g}_2|\rangle\sqrt{|U^T|} \\ &= \sqrt{\left|\left(A_1^T U^* A_2^* + B_1^T U B_2^*\right)U^T\right|}.\end{aligned} \tag{29}$$

This is (2.13) in [15] (with missing equation number), whence the first expression in (25) is a special case. For $g_1 = g_2$ it is (34) in [26] except that there the factor $\sqrt{|U^T|}$ gets lost in the derivation from the preceding equation (33).

IV. FORMULA OF ONISHI AND YOSHIDA

Ring and Schuck call $\langle g|\rangle = \sqrt{|A|}$ or the second expression in (25) the "Onishi formula" [16], referring to the paper [14] by Onishi and Yoshida. As noted in the Introduction, the formula actually written by Onishi and Yoshida is quite different. First of all, these authors consider not the state $|g\rangle$ but the state

$$|\tilde{g}\rangle = \frac{|g\rangle}{\langle|g\rangle}. \tag{30}$$

This state has no sign ambiguity; the arbitrary sign in $|g\rangle$ cancels out in the division. The state $|\tilde{g}\rangle$ can be defined alternatively by $(ga_i)|\tilde{g}\rangle = 0$ and the normalization $\langle|\tilde{g}\rangle = 1$ (which implies that generally $\langle\tilde{g}|\tilde{g}\rangle > 1$). The uniqueness of $|\tilde{g}\rangle$ comes at the cost of a lack of generality; $|\tilde{g}\rangle$ is undefined when $\langle|g\rangle = 0$. From another point of view, when G is written as in (11), the maximal neighborhood of 1 where $\langle|g\rangle \neq 0$ is described by $y_i < \pi/2$ for every y_i in (22), and this set is simply connected. Bally and Duguet introduce in their formalism [12] a similar limitation by demanding that, for all Bogolyubov transformations g to be considered, the amplitudes $\langle|\mathrm{vac}(g)\rangle$ have equal phases, where $|\mathrm{vac}(g)\rangle$ is the quasifermion vacuum state assigned to g. This condition clearly fails when $\langle|\mathrm{vac}(g)\rangle = 0$.

Onishi and Yoshida consider the case when every g is unitary and proper, and express $|\tilde{g}\rangle$ by its Thouless expansion [27]

$$|\tilde{g}\rangle = \exp \tfrac{1}{2} a_-^\dagger F a_|^\dagger\, |\rangle, \tag{31}$$

where the skew symmetric matrix F is related to the matrices A and B in (24) by $F = (BA^{-1})^*$ [28] (which shows once more way that $|\tilde{g}\rangle$ is undefined when $|A| = 0$). They hence derive

$$\langle\tilde{g}_1|\tilde{g}_2\rangle = \exp \tfrac{1}{2}\,\mathrm{tr}\log(1 + F_1^\dagger F_2). \tag{32}$$

(To be accurate, in their formula, the second term in the argument of the logarithm is $F_2 F_1^\dagger$, but this makes no difference due to the trace.) Notably, Onishi and Yoshida do not show their derivation. The short derivation below makes repeated use of the relation

$$\left[a_|, \exp \tfrac{1}{2} a_-^\dagger F a_|^\dagger\right] = F a_|^\dagger \exp \tfrac{1}{2} a_-^\dagger F a_|^\dagger, \tag{33}$$

which is mentioned in their paper.

What must be proven is that, for any two skew symmetric matrices P and Q, the identity

$$\begin{aligned}\omega &:= \langle| \exp \tfrac{1}{2} a_- P a_|\, \exp \tfrac{1}{2} a_-^\dagger Q a_|^\dagger |\rangle \\ &= \exp \tfrac{1}{2}\,\mathrm{tr}\log(1 + PQ)\end{aligned} \tag{34}$$

holds. With

$$f(z) := \langle| \exp \tfrac{1}{2} z a_- P a_|\, \exp \tfrac{1}{2} a_-^\dagger Q a_|^\dagger |\rangle, \tag{35}$$

one gets

$$\begin{aligned}
f'(z) &= \frac{1}{2}\left\langle\left|\left(\exp\frac{1}{2}za_-Pa_|\right)a_-Pa_| \exp\frac{1}{2}a_-^\dagger Q a_|^\dagger\right|\right\rangle \\
&= \frac{1}{2}\left\langle\left|\left(\exp\frac{1}{2}za_-Pa_|\right)a_-PQa_|^\dagger \exp\frac{1}{2}a_-^\dagger Q a_|^\dagger\right|\right\rangle \\
&= \frac{1}{2}\left\langle\left|\left(\exp\frac{1}{2}za_-Pa_|\right)\right.\right. \\
&\qquad \left.\left.\times\,(\mathrm{tr}\,PQ - a_-^\dagger QPa_|)\exp\frac{1}{2}a_-^\dagger Q a_|^\dagger\right|\right\rangle \\
&= \frac{1}{2}\left\langle\left|\left(\exp\frac{1}{2}za_-Pa_|\right)\right.\right. \\
&\qquad \left.\left.\times\,(\mathrm{tr}\,PQ - za_-PQPa_|)\exp\frac{1}{2}a_-^\dagger Q a_|^\dagger\right|\right\rangle \\
&= \frac{1}{2}\left\langle\left|\left(\exp\frac{1}{2}za_-Pa_|\right)\right.\right. \\
&\qquad \left.\left.\times\,(\mathrm{tr}\,PQ - za_-PQPQa_|^\dagger)\exp\frac{1}{2}a_-^\dagger Q a_|^\dagger\right|\right\rangle \\
&= \frac{1}{2}\left\langle\left|\left(\exp\frac{1}{2}za_-Pa_|\right)\right.\right. \\
&\qquad \times\,(\mathrm{tr}(PQ - zPQPQ) + za_-^\dagger QPQPa_|) \\
&\qquad \left.\left.\times\,\exp\frac{1}{2}a_-^\dagger Q a_|^\dagger\right|\right\rangle \\
&= \cdots \\
&= \frac{1}{2}\,\mathrm{tr}(PQ - zPQPQ + z^2 PQPQPQ - \cdots) \\
&\qquad \times\left\langle\left|\exp\frac{1}{2}za_-Pa_| \exp\frac{1}{2}a_-^\dagger Q a_|^\dagger\right|\right\rangle \\
&= \frac{1}{2}\,\mathrm{tr}\,PQ(1 + zPQ)^{-1} f(z) \\
&= \left(\frac{d}{dz}\frac{1}{2}\,\mathrm{tr}\log(1 + zPQ)\right) f(z).
\end{aligned} \tag{36}$$

Since $f(0) = 1$, there follows

$$f(z) = \exp \tfrac{1}{2}\,\mathrm{tr}\log(1 + zPQ) \tag{37}$$

and (34), in particular, provided one takes $\log 1 = 0$.

This argument requires that the Taylor expansion of $(1 + zPQ)^{-1}$ converges. This holds when z is numerically less than the reciprocal of every nonzero characteristic root of PQ. However, because the expansion of $\exp \frac{1}{2} z a_- P a_|$ on powers z^n terminates when $2n > d$, the function f is a polynomial.

Therefore, by analytic continuation, despite its nominal multi-valuedness, the right-hand side of (37) is single-valued outside the singularities of the logarithm, which occur when z equals minus the reciprocal of a characteristic root, and it can be extended to the singularities so as to be defined for every z as a continuous function of z. It follows by a similar argument that the right-hand side of (34) is well defined as a continuous function of the entries of P and Q.

In terms of the characteristic roots r_i of PQ, the expression (37) can be written

$$f(z) = \exp \frac{1}{2} \sum_i \log(1 + zr_i) = \sqrt{\prod_i (1 + zr_i)}, \qquad (38)$$

where one must take $\sqrt{1} = 1$ and for $z \neq 0$ choose the sign of the square root that makes it continuous in z. Since f is a polynomial, the square root is a polynomial in z, so the characteristic roots have even multiplicities [15]. The only assumption was that P and Q be skew symmetric, so this property of the spectrum of characteristic roots must hold, in fact, for every product of two skew symmetric complex matrices. This can be shown more directly as follows. Cayley proved that the determinant of a skew symmetric matrix S can be written as the square of a polynomial in its entries which he called its Pfaffian, and which is denoted usually by pf S [29,30]. Hence, when P and Q are skew symmetric, one has

$$\begin{aligned} |1 + zPQ| &= \begin{vmatrix} 1 + zPQ & -zP \\ 0 & 1 \end{vmatrix} = \begin{vmatrix} zP & 1 \\ -1 & Q \end{vmatrix} \begin{vmatrix} Q & -1 \\ 1 & 0 \end{vmatrix} \\ &= \begin{vmatrix} zP & 1 \\ -1 & Q \end{vmatrix} = \left[\operatorname{pf} \begin{pmatrix} zP & 1 \\ -1 & Q \end{pmatrix} \right]^2, \end{aligned} \qquad (39)$$

which implies that the nonzero characteristic roots of PQ have even multiplicities. Yet another proof of this result was given by Oi, Mizusaki, Shimizu, and Sun under some restricting assumptions [31]. Using it, one can express the right-hand side of (34) as

$$\prod\nolimits_i' (1 + r_i), \qquad (40)$$

where one out of every pair of equal characteristic roots of PQ, counted with multiplicity, is included in the product. This reduces the calculation of $\langle \tilde{g}_1 | \tilde{g}_2 \rangle$ to the determination of the characteristic roots of $F_1^\dagger F_2$ [15].

In [26,28], the expression (32) is written

$$\langle \tilde{g}_1 | \tilde{g}_2 \rangle = \sqrt{|1 + F_1^\dagger F_2|}. \qquad (41)$$

In part of the literature, (32) or variants such as (41), where the right-hand side is well defined by continuity, but whose scope was seen to be limited to a neighborhood of 1, are called the "Onishi formula" [8–13]. Mizusaki, Oi, and Shimizu derived (41) from the linked cluster theorem [11], and Porro and Duguet obtained (32) by a diagrammatic method [13].

V. ROBLEDO FORMULA

The definition of the Pfaffian of a $2d$-dimensional skew symmetric matrix S with entries s_{ij} can be written

$$\operatorname{pf} S = \sum_\pi \operatorname{sgn} \begin{pmatrix} 1 & 2 & \dots & 2d \\ i_1 & i_2 & \dots & i_{2d} \end{pmatrix} \prod_{\text{odd } \nu < 2d} s_{i_\nu i_{\nu+1}}, \qquad (42)$$

where the sum runs over partitions $\pi = \{\{i_1, i_2\}, \dots, \{i_{2d-1}, i_{2d}\}\}$ of $\{1, 2, \dots, 2d\}$ [29]. Hence,

$$\operatorname{pf} \begin{pmatrix} 0 & 1 \\ -1 & Q \end{pmatrix} = (-1)^{d(d-1)/2} \qquad (43)$$

because in this case the product in (42) is different from 0 only when $\pi = \{\{1, d+1\}, \{2, d+2\}, \dots, \{d, 2d\}\}$. Writing the right-hand side of (37) as in (41), one gets from (39) that

$$f(z) = \sqrt{|1 + zPQ|} = (-)^{d(d-1)/2} \operatorname{pf} \begin{pmatrix} zP & 1 \\ -1 & Q \end{pmatrix} \qquad (44)$$

with the correct sign due to (43). For $z = 1$, this becomes

$$\omega = (-)^{d(d-1)/2} \operatorname{pf} \begin{pmatrix} P & 1 \\ -1 & Q \end{pmatrix}, \qquad (45)$$

where ω is defined in (34). In a slightly different but equivalent form, this identity was proved by Robledo [7] by means of Berezin integration [32]. Pfaffians can be calculated by Householder transformation [33], which may be numerically more stable than determining the characteristic roots of an arbitrary complex matrix [7]. The matrix in (45) is seen to have twice the dimension of that PQ. Other derivations of (45) are given by Mizusaki, Oi, and Shimizu [11] and Porro and Duguet [13]. I give yet another, combinatoric, proof.

Denoting the entries of P and Q by p_{ij} and q_{ij}, one can write

$$\begin{aligned} \exp \frac{1}{2} a_- P a_| &= \sum_{\pi_1} \operatorname{sgn} \begin{pmatrix} k_1 & k_2 & \dots & k_{2m_1} \\ i_1 & i_2 & \dots & i_{2m_1} \end{pmatrix} \\ &\quad \times \prod_{\text{odd } \nu < 2m_1} p_{i_\nu i_{\nu+1}} a_{i_\nu} a_{i_\nu+1}, \\ \exp \frac{1}{2} a_-^\dagger Q a_|^\dagger &= \sum_{\pi_2} \operatorname{sgn} \begin{pmatrix} l_1 & l_2 & \dots & l_{2m_2} \\ j_1 & j_2 & \dots & j_{2m_2} \end{pmatrix} \\ &\quad \times \prod_{\text{odd } \nu < 2m_2} q_{j_\nu j_{\nu+1}} a_{j_\nu}^\dagger a_{j_\nu+1}^\dagger, \end{aligned} \qquad (46)$$

where the sums run over partitions $\pi_1 = \{\{i_1, i_2\}, \dots, \{i_{2m_1-1}, i_{2m_1}\}\}$ and $\pi_2 = \{\{j_1, j_2\}, \dots, \{j_{2m_2-1}, j_{2m_2}\}\}$ of even subsets $\{k_1, k_2, \dots, k_{2m_1}\}$ and $\{l_1, l_2, \dots, l_{2m_2}\}$ of $\{1, 2, \dots, d\}$, and $k_1 < k_2 < \dots < k_{2m_1}$ and $l_1 < l_2 < \dots < l_{2m_2}$. Inserting these expressions into the definition of ω in (34) gives

$$\begin{aligned} \omega &= \sum_{\pi_1 \sim \pi_2} \operatorname{sgn} \begin{pmatrix} i_1 & i_2 & \dots & i_{2m} \\ j_1 & j_2 & \dots & j_{2m} \end{pmatrix} \\ &\quad \times \prod_{\text{odd } \nu < 2m} p_{i_\nu i_{\nu+1}} q_{j_{\nu+1} j_\nu}, \end{aligned} \qquad (47)$$

where $\pi_1 \sim \pi_2$ is shorthand for $\{i_1, i_2, \dots, i_{2m_1}\} = \{j_1, j_2, \dots, j_{2m_2}\}$, which implies $m_1 = m_2 := m$. Next notice that $(-)^{d(d-1)/2}$ is the signature of the simultaneous permutation of the rows and the columns that transforms the matrix in (45) into the $d \times d$ block matrix S with diagonal blocks

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{48}$$

and off-diagonal blocks

$$\begin{pmatrix} p_{ij} & 0 \\ 0 & q_{ij} \end{pmatrix}, \tag{49}$$

so, by (42), the identity (45) can be written

$$\omega = \operatorname{pf} S. \tag{50}$$

I set out to calculate pf S.

The pairs $\{i_\nu, i_{\nu+1}\}$ in (42) can be so chosen that always $i_\nu < i_{\nu+1}$. Then, when a factor $s_{i_\nu i_{\nu+1}}$ stems from a submatrix (48), it equals 1, so one can omit these factors from the product and the corresponding columns from the permutation symbol, which does not alter the signature. When $s_{i_\nu i_{\nu+1}}$ is p_{ij}, then i_ν and $i_{\nu+1}$ are odd, and when $s_{i_\nu i_{\nu+1}}$ is q_{ij}, then i_ν and $i_{\nu+1}$ are even. Since equally many odd and even indices remain after the factors from the diagonal submatrices were removed, the product has equally many factors p_{ij} and q_{ij}. I denote by m this number, which takes the values of the variable m in (47), the integral values from 0 to $\lfloor d/2 \rfloor$. The general term in (42) now is

$$\operatorname{sgn}\begin{pmatrix} 2k_1-1 & 2k_1 & 2k_2-1 & \dots & 2k_{2m} \\ i_1 & i_2 & i_3 & \dots & i_{4m} \end{pmatrix} \prod_{\text{odd } \nu < 4m} s_{i_\nu i_{\nu+1}}, \tag{51}$$

where $1 \leqslant k_1 < k_2 < \cdots < k_{2m} \leqslant d$, and for every ν the indices i_ν and $i_{\nu+1}$ are either both odd or both even. For a given m, the sum runs over all such ordered sets $(k_i \mid i = 1 \dots 2m)$ and all partitions of $\{2k_1-1, 2k_1, 2k_2-1, \dots, 2k_{2m}\}$ into such pairs $\{i_\nu, i_{\nu+1}\}$.

A sequence of cyclic permutations of odd length changes the sequence in the upper row of the permutation symbol in (51) into $2k_1-1, 2k_2-1, \dots, 2k_{2m}-1, 2k_{2m}, \dots, 2k_2, 2k_1$. This leaves the signature unaltered. Also without changing the signature, one can reorder the pairs $\{i_\nu, i_{\nu+1}\}$ in the lower row so that all the pairs with odd i_ν and $i_{\nu+1}$ appear before the pairs with even i_ν and $i_{\nu+1}$. Flipping i_ν and $i_{\nu+1}$ in the latter pairs is equivalent to replacing every q_{ij} by q_{ji}. After these permutations, one can write the entries in the first half of the lower row of the permutation symbol in the form $2i_1-1, 2i_2-1, \dots, 2i_m-1$ and the entries in the second half of that row in the form $2j_m, \dots, 2j_2, 2j_1$. The signature in (51) thus becomes

$$\operatorname{sgn}\begin{pmatrix} k_1 & k_2 & \cdots & k_{2m} \\ i_1 & i_2 & \cdots & i_{2m} \end{pmatrix} \operatorname{sgn}\begin{pmatrix} k_1 & k_2 & \cdots & k_{2m} \\ j_1 & j_2 & \cdots & j_{2m} \end{pmatrix} = \operatorname{sgn}\begin{pmatrix} i_1 & i_2 & \cdots & i_{2m} \\ j_1 & j_2 & \cdots & j_{2m} \end{pmatrix}, \tag{52}$$

and the product becomes

$$\prod_{\text{odd } \nu < 2m} p_{i_\nu i_{\nu+1}} q_{j_{\nu+1} j_\nu}. \tag{53}$$

Since both sets $\{\{i_1, i_2\}, \{i_3, i_4\}, \dots, \{i_{2m-1}, i_{2m}\}\}$ and $\{\{j_1, j_2\}\{j_3, j_4\}, \dots, \{j_{2m-1}, j_{2m}\}\}$ take the values of all partitions of a common even subset of $\{1, 2, \dots, d\}$ into pairs, by comparison with (47), one arrives at (50).

VI. SUMMARY

The representation of a Bogolyubov transformation of fermion annihilation and creation operators on the Fock space related to a finite-dimensional space of single-fermion states was discussed from the point of view of its equivalence to a spin representation of an orthogonal group. It was shown, in particular, that a much discussed "sign problem of the Onishi formula" can be traced back to the double-valuedness of spin representations. The sign ambiguity referred to by this language affects a formula for the overlap amplitude between two quasifermion vacua in the much cited book by Ring and Schuck and some related formulas but not the original formula of Onishi and Yoshida, whose is scope is, however, more limited. Derivations based on the interpretation of the Fock space representation as a spin representation were shown for the formula of Ring and Schuck and some related formulas. In some cases, these derivations are more complete than those in the literature. I gave a short proof of the formula of Onishi and Yoshida, whose derivation is missing in their paper, based on a relation written there, and a new, combinatoric proof of an equivalent formula recently derived by Robledo.

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