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Para-Fermi algebras and the many-electron correlation problem

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A new formulation of the many-electron correlation problem is presented based on the use of parastatistics. It is shown that second-order para-Fermi creation and annihilation operators, which correspond to the creation and annihilation of spin-averaged paraparticles, occur naturally for the spin-independent many-electron problem. Moreover, the spin-independent many-electron Hamiltonian is directly expressible in terms of the parafield operators. The structure of the general para-Fermi algebra is also investigated from the viewpoint of the pseudo-orthogonal group $O(2n+1,1)$. Finally, an explicit matrix representation for the para-Fermi algebra of order 2, which enables one to handle even particle-number-nonconserving operators, is obtained in a canonical $U(n)$-adapted basis.

I. INTRODUCTION

In this paper we investigate the spin-independent many-electron correlation problem. Currently, one of the most often used techniques in going beyond the Hartree-Fock approximation, at least for atomic and molecular systems, is the well-known shell model or configuration-interaction (CI) approach. This is not only due to its conceptual simplicity, its universality, and the developments in computing technology, but also due to certain methodological advances which made it possible to perform large-scale CI computations and thus to partially overcome a slow convergence of this procedure. One particularly successful development in this respect is currently known as the unitary group approach (UGA).[1–3] It is based on earlier developments in the nuclear many-body problem due to Moshinsky[4] as well as on relatively recent advances in the representation theory of compact Lie groups.[5,6] It may also be regarded as an outgrowth of the spin-free formulation due to Matsen.[7]

The UGA to the many-electron correlation problem exploits the fact that the spin-independent many-electron Hamiltonian is expressible as a bilinear form in the orbital (or spin-free) $U(n)$ generators. This enables one to develop efficient methods for Hamiltonian matrix-element evaluation using known[2,8] matrix-element formulas for the $U(n)$ generators. This latter problem dates back to the original work of Gelfand and Tsetlin[5] and Baird and Biedenharn,[6] who developed explicit formulas for the matrix elements of $U(n)$ generators in the Gelfand-Tsetlin basis of any irreducible representation of $U(n)$ (see also Ref. 9). The general formalism of Refs. 5, 6, and 9 considerably simplifies for the many-electron problem since only the representations of $U(n)$ with at most two columns in the Young tableau need be considered. This simplification, first exploited by Paldus,[1,2] together with its graphical representation due to Shavitt,[3] has led to the development of numerous computational implementations ranging from the integral-driven,[10] loop-driven,[11] shape,[12] or internal interaction block-driven[13] approach to matrix-element-driven approach[14] based on harmonic level excitation diagrams.[15]

It is our aim here to investigate the many-electron correlation problem from the viewpoint of parastatistics, first introduced by Green[16] as a general scheme of quantization which includes normal Fermi and Bose statistics as a special case. This generalized method of field quantization has been made the subject of numerous investigations[17–20] since its inception.[16] However, Greenberg and Messiah[20] have shown that no presently known particle can be para. In spite of Nature's apparent preference for Fermi or Bose statistics, there has come an increasing appreciation of the structure of para-Bose and para-Fermi algebras. It was shown by Kamefuchi and Takahashi[21] and Ryan and Sudarshan[22] that all unitary irreducible representations of the para-Fermi (or para-Bose) algebra correspond to unitary representations of the orthogonal (or symplectic) group. Not all such representations are appropriate to the description of paraparticles since we are usually restricted to the (unique) Fock-space representation which, in the case of the para-Fermi algebra of order p, as discussed in this paper, corresponds to the pth spinor representation of the orthogonal group $O(2n+1)$. The Fock-space representations of these algebras have been investigated in the para-Bose case by Alabiso, Duimio, and Redondo[23] and in the para-Fermi case by Bracken and Green.[24] The representations of these algebras have also been analyzed from the viewpoint of the symmetric group by Ohnuki and Kamefuchi.[25] General results on realizations of Lie algebras in terms of parafield operators and interrelationships between representations of parafield operators of different types have been obtained by Kademova *et al.*[26] A detailed account of parastatistics and its applications in quantum field theory can be found in Refs. 18 and 27.

This paper is an extension of an earlier investigation[28] in which we demonstrated that the recently introduced Clifford algebra UGA (CAUGA) formalism[29] may be described in terms of the para-Fermi algebra. In this paper it is demonstrated, using the ansatz originally proposed by Green,[16] that parafermions of order 2 may be explicitly constructed for the spin-independent many-electron problem. The parafermion creation operators may be interpreted as creating a spin-averaged paraparticle. Moreover, it is shown that the spin-independent many-electron Hamiltonian is expressible as a bilinear form in the U(n) generators which occur as those second-order operators in the para-Fermi algebra preserving the number of paraparticles. In this sense it is seen that parafermions of order 2 occur naturally for the spin-independent many-electron correlation problem. The states of such a system may then be expressed as a polynomial in the para-Fermi creation operators acting on the vacuum state. This procedure thereby affords an alternative spin-independent approach to the molecular correlation problem and opens up the possibility of exploiting previous work on para-Fermi algebras.

In our approach we find it both convenient and natural to introduce the pseudo-orthogonal group O($2n+1,1$) into the para-Fermi algebra. It transpires that the "statistical quantum number" of Ohnuki and Kamefuchi,[25] which occurs as an O($2n$) labeling invariant in the work of Bracken and Green,[24] corresponds to a Cartan generator of the group O($2n+1,1$). This procedure thereby affords a generalization of Bracken and Green's work to certain non-Fock-space representations. We note, in this connection, that non-Fock-space representations for parafermions of order 2 and the introduction of a pseudo-orthogonal group O($2n+1,1$) (which is different from the one used in this paper) were considered by Carey[19] in his investigation on the leptons.

We should also note that the formalism developed in this paper may be extended to other quantum-mechanical systems of interest in physics. For example, in treating spin- and isospin-independent interactions in nuclear physics, parafermions of order 4 naturally appear. The work of this paper may also be extended to many-boson problems, in which case one is concerned with the appropriate para-Bose algebra and representations of the symplectic group. We mention also the possibility of treating composite systems of bosons and fermions, which occur, for example, in investigating vibronic modes in molecules or Fröhlich's electron-phonon interaction in solids, where Lie superalgebras[30] will naturally occur. Finally, we note that effective algorithms for matrix-element evaluation of the O($2n+1$) generators [in a U(n)-adapted basis] might be of use in treating particle nonconserving operators, which are required to handle various electron attachment or detachment processes such as simple or multiple ionization or electron capture phenomena. In our approach, this latter problem is equivalent to that of obtaining a matrix representation of the parafield operators in a U(n) basis. This problem is considered, in the Fock-space representation, for parafermions of order 2 in Sec. V.

The paper is set up as follows. The structure of the general para-Fermi algebra is outlined in Sec. II and the pseudo-orthogonal group O($2n+1,1$) is introduced in Sec. III. A parastatistical approach to the spin-independent many-electron problem is then developed in Sec. IV. The concluding Sec. V gives a matrix representation for the parafermion algebra of order 2 in a U(n)-adapted basis as already mentioned.

II. PARA-FERMI ALGEBRA OF ORDER p

The annihilation operators a_i and creation operators $a^i=a^\dagger_i$ ($i=1,\ldots,n$) for parafermions of arbitrary order satisfy[16]

$$\begin{aligned} &[a_i,[a_j,a_k]]=0\ ,\\ &[a_i,[a^j,a_k]]=2\delta^j{}_i a_k\ ,\\ &[a_i[a^j,a^k]]=2(\delta^j{}_i a^k-\delta^k{}_i a^j)\ , \end{aligned} \tag{1}$$

as well as relations conjugate to these.

The irreducible (unitary) representations of the para-Fermi algebra (1) are known[24] to correspond to finite-dimensional irreducible representations of the orthogonal group O($2n+1$). To see this, we define para-Fermi operators a_ρ for $\rho=1,\ldots,2n$ according to

$$a_{\bar{i}}=a^i,\quad \bar{i}=i+n,\quad i=1,\ldots,n\ .$$

We then introduce the O($2n$) metric $g_{\rho\sigma}$ defined by

$$g_{\rho\sigma}=g_{\sigma\rho}=\begin{cases}1 & \text{if } |\rho-\sigma|=n\\ 0 & \text{otherwise}\ .\end{cases} \tag{2}$$

If $g^{\rho\sigma}$ ($=g_{\rho\sigma}$) denotes the inverse metric, we may raise and lower indices according to

$$a^\rho=g^{\rho\sigma}a_\sigma,\quad a_\rho=g_{\rho\sigma}a^\sigma\ ,$$

etc. In this notation the para-Fermi defining relations, Eq. (1), may be expressed in a unified notation as follows:

$$[a_\rho,[a_\mu,a_\nu]]=2(g_{\rho\mu}a_\nu-g_{\rho\nu}a_\mu)\ . \tag{3}$$

It now easily follows that the operators

$$\alpha_{\mu\nu}=\tfrac{1}{2}[a_\mu,a_\nu] \tag{4}$$

satisfy the relations

$$[\alpha_{\mu\nu},a_\rho]=g_{\rho\nu}a_\mu-g_{\rho\mu}a_\nu\ , \tag{5a}$$

$$[\alpha_{\mu\nu},\alpha_{\rho\sigma}]=g_{\nu\rho}\alpha_{\mu\sigma}+g_{\mu\sigma}\alpha_{\nu\rho}-g_{\mu\rho}\alpha_{\nu\sigma}-g_{\nu\sigma}\alpha_{\mu\rho}\ , \tag{5b}$$

similarly as in the CAUGA [cf. Eqs. (11) and (5) of Ref. 29], so that the operators $\alpha_{\mu\nu}$, Eq. (4), constitute the generators of the group O($2n$) whilst the operators

$$\alpha_{\mu\nu},\quad a_\rho/\sqrt{2} \tag{6}$$

constitute the generators of the group O($2n+1$). It follows, therefore, that the (unitary) irreducible representations of the para-Fermi algebra are to comprise finite-dimensional irreducible representations of the group O($2n+1$) with infinitesimal generators (6).

The Fock-space representation is characterized as that representation which admits a unique vacuum state $|0\rangle$ defined by the conditions

$$a_i\,|0\rangle=0,\quad i=1,\ldots,n\ . \tag{7a}$$

It may be shown[20] that the vacuum state $|0\rangle$ must also satisfy the conditions

$$a_i a^j |0\rangle = p\delta^j{}_i |0\rangle , \quad (7b)$$

for some positive integer p, which is called the *order* of the parastatistics. Thus, for parastatistics of a given order p there exists a unique Fock-space representation: This is the representation of interest in physical applications. It is important to note that in addition to the relations (3), parafermions obey extra relations which depend on the order p of the statistics. For example, parafermions of order p always satisfy the conditions

$$a_p{}^{p+1}=0$$

as well as additional relations which may be found in the work of Bracken and Green.[24] We note that parafermions of order 1 correspond to normal fermions.

Throughout this paper, unless otherwise stated, we shall be working in the Fock-space representation for parastatistics of a fixed order p, i.e., we assume the existence of a unique vacuum state $|0\rangle$ satisfying Eqs. (7a) and (7b). The corresponding Hilbert space of para-Fermi states (i.e., the parafermion Fock space), herein denoted $\mathcal{F}_p$, is given by all polynomials in the para-Fermi creation operators acting on the vacuum state $|0\rangle$.

As a Cartan subalgebra of $O(2n+1)$ [and $O(2n)$] we choose the operators

$$h_i = \alpha^i{}_i = \alpha_{\bar{i}i}, \quad i=1,\ldots,n$$

which serve to uniquely label the weights of $O(2n+1)$. It is easily seen[24] that the vacuum state $|0\rangle$ constitutes a (unique) minimal weight state of $O(2n+1)$ weight:

$$(-p/2,-p/2,\ldots,-p/2) .$$

It thus follows that the space of para-Fermi states $\mathcal{F}_p$ is to constitute the irreducible representation of $O(2n+1)$ with highest weight:

$$(p/2,p/2,\ldots,p/2) .$$

The particle-number-conserving operators $b^i{}_j$,

$$b^i{}_j = \tfrac{1}{2}[a^i,a_j] ,$$

form the generators of the unitary subgroup $U(n)$ of $O(2n)$. However, following Bracken and Green,[24] we shall work instead with the shifted $U(n)$ generators

$$E^i{}_j = \tfrac{1}{2}[a^i,a_j] + \tfrac{1}{2}p\delta^i{}_j , \quad (8)$$

where p is the order of the parastatistics. The Fock space $\mathcal{F}_p$ possesses the remarkable property that it decomposes into a direct sum of irreducible representations of $U(n)$ with highest weights of the form $\lambda=(\lambda_1,\lambda_2,\ldots,\lambda_n)$ where

$$p \ge \lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n \ge 0 \quad (9)$$

and all such representations occur exactly once.[24,25] In other words, all irreducible representations of $U(n)$ with no more than p columns in the Young tableau occur in $\mathcal{F}_p$ with unit multiplicity.

The Fock space also decomposes into a direct sum of irreducible representations of $O(2n)$ with highest weights

$$\Lambda_q = (p/2,p/2,\ldots,p/2,p/2-q), \quad 0 \le q \le p .$$

The irreducible representations of $U(n)$ occurring in the $O(2n)$ representation with the highest weight Λ_q have highest weights λ satisfying Eq. (9) and the additional condition[24]

$$\tilde{q} = -\sum_{i=1}^{n}(-1)^i\lambda_i , \quad (10a)$$

where

$$\tilde{q} = \begin{cases} q & \text{for } n \text{ even} \\ p-q & \text{for } n \text{ odd} . \end{cases} \quad (10b)$$

The $O(2n)$ invariant $\tilde{q}$ is the statistical quantum number appearing in the work of Ohnuki and Kamefuchi.[25]

The group $O(2n)$ admits the second-order Casimir invariant (the summation convention over repeated indices is now implied)

$$\sigma_2 = \alpha^\rho{}_\tau \alpha^\tau{}_\rho ,$$

which takes a constant value in the irreducible representation with highest weight Λ_q given by[24]

$$\sigma_2 = pn(n+p/2-1) - 2\Delta , \quad (11)$$

where

$$\Delta = q(p-q) = \tilde{q}(p-\tilde{q}) . \quad (12)$$

The group $O(2n+1)$ also admits a second-order Casimir invariant

$$\hat{\sigma}_2 = \sigma_2 + \tfrac{1}{2}\{a_\rho,a^\rho\} ,$$

which has an eigenvalue given by[24]

$$\hat{\sigma}_2 = pn(n+p/2) . \quad (13)$$

We note that the operator Δ of Eq. (12) may be alternatively expressed as

$$\Delta = \tfrac{1}{4}\{a_\rho,a^\rho\} - \tfrac{1}{2}np ,$$

which is equivalent to

$$\tfrac{1}{2}\{a_\rho,a^\rho\} = \hat{\sigma}_2 - \sigma_2 = 2\Delta + np . \quad (14)$$

Although the operator $\tilde{q}$ of Eq. (10) is an $O(2n)$ invariant, it is not an invariant of $O(2n+1)$. In fact, the creation or annihilation operator a^σ can only increase or decrease one of the weights by one unit and may thus be separated into the vector operators $a^\sigma{}_+$ and $a^\sigma{}_-$ of $O(2n)$ which, respectively, increase and decrease the eigenvalue $\tilde{q}$ by one unit, so that

$$a^\sigma = a^\sigma{}_+ + a^\sigma{}_-$$

and

$$[\tilde{q},a^\sigma{}_\pm] = \pm a^\sigma{}_\pm ,$$

so that

$$[\tilde{q},a^\sigma] = a^\sigma{}_+ - a^\sigma{}_- . \quad (15)$$

The $a^\sigma{}_\pm$ may be explicitly constructed using the relations[24]

$$\alpha^\sigma{}_\rho a^\rho{}_\pm = (n-1 \pm \tfrac{1}{2}\Pi) a^\sigma{}_\pm ,$$

where

$$\tfrac{1}{2}\Pi=\tilde{q}-p/2 \; . \tag{16}$$

Following Bracken and Green[24] we set

$$b^{\rho}=a^{\rho}{}_{+}, \quad c^{\rho}=a^{\rho}{}_{-} \tag{17}$$

and note that these operators satisfy the Hermiticity condition

$$(b^{\rho})^{\dagger}=c_{\rho}=g_{\rho\sigma}c^{\sigma} \; .$$

It may be directly shown, with some work,[24] that the operators (17) satisfy the commutation relations

$$\begin{aligned} &[b^{\rho},b^{\sigma}]=[c^{\rho},c^{\sigma}]=0 \; , \\ &[b^{\rho},c^{\sigma}]=-[b^{\sigma},c^{\rho}]=\alpha^{\rho\sigma} \; , \end{aligned} \tag{18}$$

where, in our previous notation, $\alpha^{\rho\sigma}=\frac{1}{2}[a^{\rho},a^{\sigma}]$. The entire para-Fermi algebra may thus be described in terms of the operators (17) and their commutation relations, Eq. (18). We shall now present an alternative description of these results in terms of the pseudo-orthogonal group $O(2n+1,1)$.

III. PSEUDO-ORTHOGONAL GROUP FORMULATION

In order to introduce the pseudo-orthogonal group $O(2n+1,1)$ we consider the Green representation[16] according to which parafermion annihilation operators are expressible as follows,

$$a_i=\sum_{\alpha=1}^{p} a^{\alpha}{}_i, \quad i=1,\ldots,n \tag{19}$$

where the $a^{\alpha}{}_i$ constitute p commuting sets of ordinary fermion annihilation operators

$$\begin{aligned} &[a^{\alpha}{}_i,a^{\beta}{}_j]=[a^{\alpha}{}_i,(a^{\dagger})^{\beta}{}_j]=0, \quad \alpha\neq\beta \\ &\{a^{\alpha}{}_i,a^{\alpha}{}_j\}=0, \quad \{a^{\alpha}{}_i,(a^{\dagger})^{\alpha}{}_j\}=\delta_{ij} \end{aligned} \tag{20}$$

together with relations conjugate to these. We note that with the Green ansatz, Eq. (19), our $U(n)$ generators $E^{i}{}_{j}$, Eq. (8), are expressible as

$$\begin{aligned} E^{i}{}_{j} &= \tfrac{1}{2}[a^{i},a_j]+\tfrac{1}{2}p\delta^{i}{}_{j} \\ &= \tfrac{1}{2}\sum_{\alpha=1}^{p}\{[(a^{\dagger})^{\alpha}{}_i,a^{\alpha}{}_j]+\delta^{i}{}_{j}\} \\ &= \sum_{\alpha=1}^{p}(a^{\dagger})^{\alpha}{}_i a^{\alpha}{}_j \; . \end{aligned} \tag{21}$$

Throughout we assume the existence of a unique vacuum state $|0\rangle$ on which all the fermion annihilation operators $a^{\alpha}{}_i$ vanish, i.e.,

$$a^{\alpha}{}_i\,|0\rangle=0, \quad \alpha=1,\ldots,p, \; i=1,\ldots,n \; . \tag{22}$$

It is easily verified that the para-Fermi operators a_{ρ} $(\rho=1,\ldots,2n)$, as defined by Eq. (19) with $a_{\bar{i}}=a^{i}=a^{\dagger}{}_i$ for $\bar{i}=i+n$ $(i=1,\ldots,n)$, satisfy the commutation relations, Eq. (3). Moreover, as a consequence of Eqs. (20) and (22), we have that

$$\begin{aligned} &a_i\,|0\rangle=0 \; , \\ &a_i a^{j}\,|0\rangle=a_i a^{\dagger}{}_j\,|0\rangle=p\delta_i{}^{j}\,|0\rangle, \quad i,j=1,\ldots,n \end{aligned}$$

as required of parastatistics of order p. This demonstrates that the Green ansatz, Eq. (19), may be employed for the Fock-space representation of parastatistics (cf. Ref. 20).

Following our previous notation we define fermion operators $a^{\alpha}{}_{\rho}$ for $\rho=1,\ldots,2n$ according to the convention

$$a^{\alpha}{}_{\bar{i}}=(a^{\dagger})^{\alpha}{}_i, \quad \bar{i}=i+n, \; i=1,\ldots,n \; .$$

With this notation, the Green ansatz, Eq. (19), may be written as follows,

$$a_{\rho}=\sum_{\alpha=1}^{p} a^{\alpha}{}_{\rho} \; ,$$

and the relations (20) may be expressed in the unified form

$$\begin{aligned} &[a^{\alpha}{}_{\rho},a^{\beta}{}_{\sigma}]=0, \quad \alpha\neq\beta \\ &\{a^{\alpha}{}_{\rho},a^{\alpha}{}_{\sigma}\}=g_{\rho\sigma} \; , \end{aligned} \tag{23}$$

where $g_{\rho\sigma}$ is the $O(2n)$ metric, Eq. (2).

We now consider the family of operators π_{α},

$$\pi_{\alpha}=\prod_{i=1}^{n}[(a^{\dagger})^{\alpha}{}_i,a^{\alpha}{}_i], \quad \alpha=1,\ldots,p \; . \tag{24}$$

The relations of Eq. (23) imply the following properties of the operators (24):

$$\begin{aligned} &\pi_{\alpha}=\pi_{\alpha}{}^{\dagger}, \quad \pi_{\alpha}{}^{2}=1 \; , \\ &\{\pi_{\alpha},a^{\alpha}{}_{\rho}\}=0, \quad [\pi_{\alpha},\pi_{\beta}]=0 \; , \\ &[\pi_{\alpha},a^{\beta}{}_{\rho}]=0, \quad \alpha\neq\beta \\ &\pi_{\alpha}\,|0\rangle=(-1)^{n}\,|0\rangle \; . \end{aligned} \tag{25}$$

It easily follows from Eqs. (23) and (25) that for each α the operators

$$\pi_{\alpha}/2, \quad a^{\alpha}{}_{\rho}/\sqrt{2}, \quad [a^{\alpha}{}_{\rho},a^{\alpha}{}_{\sigma}]/2, \quad [\pi_{\alpha},a^{\alpha}{}_{\rho}]/2\sqrt{2} \tag{26}$$

satisfy the commutation relations of an $O(2n+1,1)$ group (see Appendix), herein denoted $O_{\alpha}(2n+1,1)$. The diagonal subgroup of the product group,

$$\bigotimes_{\alpha=1}^{p} O_{\alpha}(2n+1,1) \; ,$$

is the $O(2n+1,1)$ group with infinitesimal generators

$$\hat{\pi}/2, \quad a_{\rho}/\sqrt{2}, \quad [a_{\rho},a_{\sigma}]/2, \quad [\hat{\pi},a_{\rho}]/2\sqrt{2} \; , \tag{27}$$

where

$$\hat{\pi}=\sum_{\alpha=1}^{p}\pi_{\alpha} \; .$$

The operator $\hat{\pi}/2$ is the [$O(2n)$-invariant] Cartan generator of $O(2n+1,1)$ (cf. Appendix). We note that the $O(2n+1,1)$ commutation relations are a direct consequence of the following relations satisfied by the operator $\hat{\pi}$ (see Appendix):

$$[[a_\rho,a_\sigma],\hat{\pi}]=0\ ,$$

$$[\hat{\pi},[\hat{\pi},a_\rho]]=4a_\rho\ , \tag{28}$$

$$[[\hat{\pi},a_\sigma],a_\rho]=2g_{\rho\sigma}\hat{\pi}\ .$$

The action of the Cartan generator $\hat{\pi}/2$ on the vacuum state $|0\rangle$ is given by

$$(\hat{\pi}/2)|0\rangle=(-1)^n(p/2)|0\rangle\ ,$$

and it is easily verified that the vacuum state $|0\rangle$ constitutes an $O(2n+1,1)$ minimal weight state of weight $(-p/2,-p/2,\ldots,-p/2,(-1)^n p/2)$. It follows from this that the Fock space $\mathscr{F}_p$ carries the irreducible representation of $O(2n+1,1)$ with highest weight $(p/2,\ldots,p/2,\pm p/2)$ for n odd (even). It is interesting to note that the operators

$$a^{\pi}{}_\rho=\tfrac{1}{2}[\hat{\pi},a_\rho]$$

also constitute a system of parafermions of order p such that

$$[a^{\pi}{}_\rho,a_\sigma]=g_{\rho\sigma}\hat{\pi}\ .$$

Since the Cartan generator $(\hat{\pi}/2)$ is an $O(2n)$ invariant, it follows from Schur's lemma that it must reduce to a scalar multiple of the identity on each of the $O(2n)$ irreducible representations occurring in $\mathscr{F}_p$. The eigenvalue of $\hat{\pi}/2$ on the irreducible representation of $O(2n)$ with highest weight $\Lambda_q=(p/2,\ldots,p/2,p/2-q)$ $(q=0,\ldots,p)$ is easily seen to be given by

$$\tfrac{1}{2}\Pi=\begin{cases}q-p/2, & n \text{ even}\\ p/2-q, & n \text{ odd}\ .\end{cases}$$

In terms of the statistical quantum number $\tilde{q}$ of Eq. (10) we may therefore write

$$\tfrac{1}{2}\Pi=\tilde{q}-p/2$$

in agreement with the notation of Eq. (16).

We conclude from this that the statistical quantum number $\tilde{q}$ of Ohnuki and Kamefuchi[25] corresponds (up to a scalar shift) with the Cartan generator $(\hat{\pi}/2)$ of $O(2n+1,1)$. Moreover, using the commutation relations, Eqs. (28), it is easily seen that the $O(2n)$ vectors defined by

$$a^{\sigma}{}_{\pm}=\tfrac{1}{2}(a^{\sigma}\pm[\hat{\pi}/2,a^{\sigma}])$$

satisfy the relations

$$[\hat{\pi}/2,a^{\sigma}{}_{\pm}]=\tfrac{1}{2}([\hat{\pi}/2,a^{\sigma}]\pm[\hat{\pi}/2,[\hat{\pi}/2,a^{\sigma}]])$$
$$=\tfrac{1}{2}([\hat{\pi}/2,a^{\sigma}]\pm a^{\sigma})\ ,$$

so that

$$[\hat{\pi}/2,a^{\sigma}{}_{\pm}]=\pm a^{\sigma}{}_{\pm}\ .$$

It thus follows that the operators $a^{\sigma}{}_{\pm}$ constitute $O(2n+1,1)$ root vectors which increase (decrease) the eigenvalue of $(\hat{\pi}/2)$ by one unit. The operators $a^{\sigma}{}_{\pm}$ clearly correspond to the $O(2n)$ shift vectors of Eq. (15). Indeed, in view of Eq. (16) we may alternatively write

$$a^{\sigma}{}_{\pm}=\tfrac{1}{2}(a^{\sigma}\pm[\tilde{q}-p/2,a^{\sigma}])$$
$$=\tfrac{1}{2}(a^{\sigma}\pm[\tilde{q},a^{\sigma}])\ ,$$

in agreement with Eq. (15). The commutation relations of Eq. (18) are then easily seen to follow from the $O(2n+1,1)$ commutation relations.

In conclusion, we note that our approach applies to any (unitary) representation of the para-Fermi algebra on which the Green ansatz, Eq. (19), holds. It is also interesting to note that the results of this section may be obtained independently of the Green ansatz, Eq. (19), by extending the para-Fermi algebra to include a self-adjoint operator $\hat{\pi}$ satisfying the relations of Eq. (28).

IV. THE MANY-ELECTRON PROBLEM AND PARASTATISTICS OF ORDER 2

In the many-electron problem, as formulated in current orbital theories, we start with $2n$ atomic or molecular spin orbitals $|i\alpha\rangle$ $(i=1,\ldots,n,\ \alpha=\pm)$, which span the one-electron space $\mathscr{V}_1$ employed and build the many-electron space as an appropriate antisymmetric component of the Nth-rank tensor product $\mathscr{V}_1{}^{\otimes N}$. In the second quantization formalism we associate with an orthonormal spin orbital basis $\{|i\alpha\rangle\}$ the fermion annihilation operators $X^{\alpha}{}_i$ and their adjoints $(X^{\dagger})^{\alpha}{}_i$ representing corresponding creators, which satisfy the anticommutation relations

$$\begin{aligned}&\{X^{\alpha}{}_i,X^{\beta}{}_j\}=\{(X^{\dagger})^{\alpha}{}_i,(X^{\dagger})^{\beta}{}_j\}=0\ ,\\ &\{X^{\alpha}{}_i,(X^{\dagger})^{\beta}{}_j\}=\delta^{\alpha\beta}\delta_{ij}\ .\end{aligned} \tag{29}$$

The spin-independent Hamiltonian H describing a given many-electron system is then expressible as a bilinear form in the (orbital) $U(n)$ generators

$$E^{i}{}_j=(X^{\dagger})^{(+)}{}_iX^{(+)}{}_j+(X^{\dagger})^{(-)}{}_iX^{(-)}{}_j\ , \tag{30}$$

namely (cf., e.g., Ref. 1)

$$H=\sum_{i,j}\langle i|\hat{z}|j\rangle E^{i}{}_j+\frac{1}{2}\sum_{i,j,k,l}(ij\,|\,kl)(E^{i}{}_jE^{k}{}_l-\delta^{k}{}_jE^{i}{}_l)\ , \tag{31}$$

where the coefficients $(ij\,|\,kl)$ are given by the two-electron integrals[1]

$$(ij\,|\,kl)=\langle i(1)k(2)|\hat{v}|j(1)l(2)\rangle\ .$$

Following our previous notation we define fermion operators $X^{\alpha}{}_\rho$, $\rho=1,\ldots,2n$, as follows:

$$X^{\alpha}{}_{\bar{i}}=(X^{\dagger})^{\alpha}{}_i,\quad \bar{i}=i+n,\ i=1,\ldots,n\ .$$

With this convention the anticommutation relations, Eqs. (29), may be rewritten as

$$\{X^{\alpha}{}_\rho,X^{\beta}{}_\sigma\}=\delta^{\alpha\beta}g_{\rho\sigma}\ ,$$

where $g_{\rho\sigma}$ is the $O(2n)$ metric, Eq. (2). In order to see the connection with parastatistics, we follow Sec. III and introduce the operators

$$\pi_\alpha=\prod_{i=1}^{n}(X^{\dagger})^{\alpha}{}_i,X^{\alpha}{}_i],\quad \alpha=\pm\ . \tag{32}$$

Then it is easily seen that the operators π_α are self-adjoint and satisfy the relations [cf. Eq. (25)]

$$\pi_\alpha{}^2=1,\ [\pi_\alpha,\pi_\beta]=0\ ,$$
$$\{\pi_\alpha,X^\alpha{}_\rho\}=0,\ [\pi_\alpha,X^\beta{}_\rho]=0,\ \alpha\neq\beta \tag{33}$$
$$\pi_\alpha|0\rangle=(-1)^n|0\rangle\ ,$$

where $|0\rangle$ designates the unique physical vacuum state.

We next examine the operator

$$\Theta=\pi_+\pi_-\ ,$$

which possesses the following properties:

$$\Theta^\dagger=\Theta,\ \Theta^2=1\ ,$$
$$\{\Theta,X^\alpha{}_\rho\}=0,\ \Theta|0\rangle=|0\rangle\ , \tag{34}$$

as may be readily verified using the relations (33). Thus, defining new creation and annihilation operators $a^\alpha{}_\rho$ (here we employ the notation of preceding sections),

$$a^{(+)}{}_\rho=X^{(+)}{}_\rho\ ,$$
$$a^{(-)}{}_i=\Theta X^{(-)}{}_i,\ a^{(-)}{}_{\bar{i}}=(a^\dagger)^{(-)}{}_i=(X^\dagger)^{(-)}{}_i\Theta\ , \tag{35}$$

we find them to satisfy the following relations:

$$\{a^\alpha{}_\rho,a^\alpha{}_\sigma\}=g_{\rho\sigma}\ ,$$
$$[a^\alpha{}_\rho,a^\beta{}_\sigma]=0,\ \alpha\neq\beta\ . \tag{36}$$

Thus, the operators $a^\alpha{}_\rho$, Eq. (35), constitute two commuting sets of fermions. It follows, therefore, in view of the Green ansatz, Eq. (19), that the operators

$$a_\rho=a^{(+)}{}_\rho+a^{(-)}{}_\rho,\ \rho=1,\ldots,2n \tag{37}$$

constitute a set of parafermion operators of order 2.

The relations, Eqs. (34), also imply that the operators π_α, Eq. (32), may be alternatively expressed in terms of the fermion operators defined by Eq. (35), namely

$$\pi_\alpha=\prod_{i=1}^{n}[(a^\dagger)^\alpha{}_i,a^\alpha{}_i],\ \alpha=\pm$$

in agreement with the notation of Eq. (24). In particular, we see that the operator $\hat{\pi}/2$, with

$$\hat{\pi}=\pi_++\pi_-\ , \tag{38}$$

constitutes the Cartan generator of the group $O(2n+1,1)$ with infinitesimal generators

$$\hat{\pi}/2,\ a_\rho/\sqrt{2},\ \alpha_{\rho\sigma}\equiv[a_\rho,a_\sigma]/2,\ [\hat{\pi},a_\rho]/2\sqrt{2}\ .$$

The operator Θ, Eq. (34), may be expressed in terms of the operator $\hat{\pi}$ according to

$$\hat{\pi}^2=2(1+\Theta)\ \text{ or }\ \Theta=\tfrac{1}{2}\hat{\pi}^2-1\ .$$

In the notation of Sec. II, the orbital $U(n)$ generators $E^i{}_j$, Eq. (30), may be expressed as

$$E^i{}_j=\tfrac{1}{2}[a^i,a_j]+\delta^i_j\ , \tag{39}$$

in agreement with Eq. (18) for parafermions of order 2 (cf., also Ref. 29). Indeed, we have in view of Eq. (21) that

$$\begin{aligned}\tfrac{1}{2}[a^i,a_j]+\delta^i_j&=(a^\dagger)^{(+)}{}_i a^{(+)}{}_j+(a^\dagger)^{(-)}{}_i a^{(-)}{}_j\\&=(X^\dagger)^{(+)}{}_i X^{(+)}{}_j+(X^\dagger)^{(-)}{}_i\Theta^2X^{(-)}{}_j\\&=(X^\dagger)^{(+)}{}_i X^{(+)}{}_j+(X^\dagger)^{(-)}{}_i X^{(-)}{}_j\ ,\end{aligned}$$

obtaining the $U(n)$ generators of Eq. (30) as required.

The above demonstrates that the spin-independent many-electron Hamiltonian may be expressed in terms of the para-Fermi operators a_ρ, Eq. (37), by virtue of Eqs. (31) and (39). The states for such a system are then given by all polynomials in the para-Fermi creation operators $a^\dagger{}_i$ acting on the vacuum state $|0\rangle$, i.e., the para-Fermi Fock space $\mathcal{F}_2$.

In this sense we see that parafermions of order 2 occur naturally in our formulation of the spin-independent many-electron problem. The para-Fermi creation operators $a^\dagger{}_i$ may be regarded as creating a spin-averaged paraparticle of type i. This allows the possibility of exploiting the structure of the second-order para-Fermi algebra. In particular, it follows from the representation theory of such algebras, as outlined in Sec. II, that all at most two-column representations of $U(n)$ occur once and exactly once in the Fock space $\mathcal{F}_2$. This implies that the only representations of $U(n)$ which are pertinent to the spin-independent many-electron problem are those with at most two columns in the Young tableau, as in other approaches.[1,31]

It should be noted that in addition to the relations (3), parafermions of order 2 also obey the relations[24]

$$a_\mu a_\rho a_\nu+a_\nu a_\rho a_\mu=2(g_{\mu\rho}a_\nu+g_{\rho\nu}a_\mu)\ , \tag{40}$$

which uniquely determine the structure of the second-order para-Fermi algebra. We may interpret Eq. (40) as the generalized Pauli principle for paraparticles. It implies, among other things, that

$$a_\mu{}^3=0\ ,$$

i.e., no more than two paraparticles of order 2 can occupy the same state.

We also note that the parafermion operators a_ρ, Eq. (37), may be alternatively expressed as

$$a_i=X^{(+)}{}_i+\tfrac{1}{2}[\Theta,X^{(-)}{}_i],\ i=1,\ldots,n$$

together with conjugate relations. It follows from symmetry in (+) and (−) labels that the operators

$$\bar{a}_i=\tfrac{1}{2}[\Theta,X^{(+)}{}_i]+X^{(-)}{}_i,\ i=1,\ldots,n$$

also constitute a system of para-Fermi annihilation operators. The above two para-Fermi algebras are clearly related by

$$\bar{a}_i=\tfrac{1}{2}[\Theta,a_i],\ i=1,\ldots,n$$

and hence give rise to the same para-Fermi Fock space $\mathcal{F}_2$ and the same $U(n)$ generators $E^i{}_j$, Eq. (30).

To recover the original set of fermion operators $X^\alpha{}_\rho$ ($\rho=1,\ldots,2n$, $\alpha=\pm$) from the parafermion operators a_ρ, Eq. (37), we can employ the following relations:

$$X^{(-)}{}_\rho=\tfrac{1}{2}\pi_-\{\pi_+,a_\rho\}=\tfrac{1}{2}\pi_+[\pi_-,a_\rho]\ ,$$
$$X^{(+)}{}_\rho=\tfrac{1}{2}\pi_-\{\pi_-,a_\rho\}=\tfrac{1}{2}\pi_+[\pi_+,a_\rho]\ ,$$

which may be verified with the help of Eqs. (33), (34), and (37). Finally, with regard to spin-dependent problems, we may recover the spin U(2) generators according to[1]

$$S_{\alpha\beta}=\tfrac{1}{4}[a^i,\pi_\alpha][\pi_\beta,a_i],\quad \alpha,\beta=\pm\ .$$

V. MATRIX REPRESENTATION OF PARA-FERMI OPERATORS IN A U(n) BASIS

Keeping in mind possible shell-model, perturbation-theory, or electron-propagator applications, particularly for open-shell problems involving particle-number-nonconserving operators,[29,32,33] we conclude in this section by obtaining a matrix representation for parafermion operators of order 2 in a U(n) canonical basis.

We assume throughout that we are working in the Fock space $\mathscr{F}_2$, corresponding to parafermions of order 2. As we have seen, $\mathscr{F}_2$ decomposes into irreducible representations of U(n) according to

$$\mathscr{F}=\bigoplus_{\substack{0\le a,b,c\le n\\ a+b+c=n}}\mathscr{V}(a,b,c)\ ,$$

where, in the notation of Ref. 8, $\mathscr{V}(a,b,c)$ denotes the carrier space for the irreducible representation of U(n) with Paldus labels[3,8,34] $[a,b,c]$, i.e., the irreducible representation of U(n) with highest weight

$$(\underbrace{2,2,\ldots,2}_{a},\underbrace{1,1,\ldots,1}_{b},\underbrace{0,0,\ldots,0}_{c})\ .$$

We choose as a basis for the space $\mathscr{F}_2$ the electronic Gelfand states[1,2] [also referred to[8,31] as Gelfand-Paldus (GP) basis states]

$$|[P]\rangle_{\tilde q}\ , \tag{41}$$

where $[P]$ denotes a U(n) Paldus tableau[3,8,31,34] (originally referred to[1,2] as an *ABC* tableau) and $\tilde q$ is the corresponding O($2n$)-invariant label of Eq. (10). It is uniquely determined by the U(n) Paldus labels $[a,b,c]$ according to

$$\tilde q=\begin{cases}0 & \text{if } a \text{ and } b \text{ are both even}\\ 1 & \text{if } b \text{ is odd}\\ 2 & \text{if } a \text{ is odd and } b \text{ is even}\ .\end{cases} \tag{42}$$

It is our aim here to derive the matrix elements of the para-Fermi operators a_ρ in the GP basis (41). This is equivalent to finding the matrix elements of the O($2n+1$) generators, in a U(n) basis, for the antisymmetric tensor representation $(1,1,\ldots,1)$.

We note that the para-Fermi creation operators $a^i=a^\dagger{}_i$ ($i=1,\ldots,n$) constitute a vector operator of U(n), whilst the annihilation operators a_i ($i=1,\ldots,n$) constitute a contragredient vector operator. Following the methods of Ref. 8 we may thus resolve the operators a^i and a_i into their U(n) shift components according to

$$\begin{aligned}a^i&=a[1]^i+a[2]^i\ ,\\ a_i&=a[1]_i+a[2]_i\ ,\end{aligned} \tag{43}$$

which alter the U(n) Paldus labels $[a,b,c]$ according to

$$\begin{aligned}&a[r]^i\colon\ [a,b,c]\to[a,b,c]+\delta_r\ ,\\ &a[r]_i\colon\ [a,b,c]\to[a,b,c]-\delta_r,\quad r=1,2\end{aligned}$$

where δ_r ($r=1,2$) denote the shifts

$$\delta_1=[0,1,-1],\quad \delta_2=[1,-1,0]\ .$$

The shift components, Eqs. (43), are given explicitly by (the summation convention is implied)

$$\begin{aligned}a[r]^i&=a^j\bar G[r]^i{}_j\ ,\\ a[r]_i&=a_jG[r]^j{}_i\ ,\end{aligned} \tag{44}$$

where

$$G[r]=\frac{E-\epsilon_{\bar r}}{\epsilon_r-\epsilon_{\bar r}},\quad \bar E^i{}_j=-E^j{}_i\ ,$$

and $\bar r$ denotes the opposite index to r, i.e.,

$$\bar r=\begin{cases}1 & \text{if } r=2\\ 2 & \text{if } r=1\ .\end{cases}$$

Further, we have adopted the notation of Ref. 8 where $\epsilon_r,\bar\epsilon_r$ denote the U(n) characteristic roots

$$\begin{aligned}&\epsilon_1=1+c,\quad \epsilon_2=n+2-a\ ,\\ &\bar\epsilon_1=n-c,\quad \bar\epsilon_2=a-1\ .\end{aligned} \tag{45}$$

The nonvanishing matrix elements of the operators $a[r]^i,a[r]_i$ in the GP basis, Eq. (41), are given by

$$\left\langle\begin{matrix}p_n+\delta_r\\ [P']\end{matrix}\middle| a[r]^i\middle|\begin{matrix}p_n\\ [P]\end{matrix}\right\rangle=\langle p_n+\delta_r||a||p_n\rangle\left\langle\begin{matrix}p_n+\delta_r\\ [P']\end{matrix}\middle| e_i;\begin{matrix}p_n\\ [P]\end{matrix}\right\rangle, \tag{46a}$$

$$\left\langle\begin{matrix}p_n-\delta_r\\ [P']\end{matrix}\middle| a[r]_i\middle|\begin{matrix}p_n\\ [P]\end{matrix}\right\rangle=\langle p_n-\delta_r||a||p_n\rangle\left\langle\begin{matrix}p_n-\delta_r\\ [P']\end{matrix}\middle| \bar e_i;\begin{matrix}p_n\\ [P]\end{matrix}\right\rangle, \tag{46b}$$

where $p_n=[a,b,c]$ denotes the U(n) Paldus labels and $[P],[P']$ are allowable Paldus tableaux for the subgroup U($n-1$). The first factor on the right-hand side of Eqs. (46a) and (46b) above is the O($2n+1$):U(n) reduced matrix element (RME) and the second factor is an ordinary U(n) vector (or contragredient vector) coupling coefficient. These latter coefficients are already known[35] so it remains to evaluate the corresponding RME's.

Following Ref. 8 we have the relations

$$\begin{aligned}a[r]^ia[r]_j&=\bar R_rP[r]^i{}_j\ ,\\ a[r]_ia[r]^j&=R_r\bar P[r]^j{}_i\ ,\end{aligned} \tag{47}$$

where $R_r,\bar R_r$ are U(n)-invariant operators whose eigenvalues determine the squares of the RME's, since

$$\begin{aligned}R_r&=|\langle p_n+\delta_r||a||p_n\rangle|^2\ ,\\ \bar R_r&=|\langle p_n-\delta_r||a||p_n\rangle|^2\ .\end{aligned} \tag{48}$$

The projection operators $P[r],\bar P[r]$ of Eqs. (47) are given explicitly by Eq. (10) of Ref. 8 according to which we may write

$$\mathrm{tr}\bar{P}[1]=\frac{c(2+b)}{(n+2-c)(1+b)},\quad \mathrm{tr}\bar{P}[2]=\frac{(n+1-a)b}{(1+a)(1+b)}\ . \tag{49}$$

Taking the trace of Eq. (47) we have the relations

$$\Gamma_r=R_r\mathrm{tr}\bar{P}[r],\quad \bar{\Gamma}_r=\bar{R}_r\mathrm{tr}P[r]\ , \tag{50}$$

where $\Gamma_r,\bar{\Gamma}_r$ denote the U(n) invariants

$$\Gamma_r=a_ia^j\bar{G}[r]^i{}_j,\quad \bar{\Gamma}_r=a^ia_jG[r]^j{}_i\ . \tag{51}$$

Thus to evaluate the RME's using Eq. (48) it suffices to evaluate the spectra of the operators $\Gamma_r,\bar{\Gamma}_r$, Eq. (51). We find it convenient to write

$$\Gamma_r=\tau_r/\xi_r\ , \tag{52}$$

where

$$\xi_r=\bar{\epsilon}_r-\bar{\epsilon}_{\bar{r}}\ ,$$
$$\tau_r=a_ia^j(-E^i{}_j-\bar{\epsilon}_{\bar{r}}\delta^i{}_j)\ .$$

Now

$$\tau_r=-a_ia^jE^i{}_j-\bar{\epsilon}_{\bar{r}}a_ia^i=(n-\bar{\epsilon}_{\bar{r}})\Phi_1-\Phi_2\ , \tag{53}$$

where

$$\Phi_1=a_ia^i,\quad \Phi_2=a_iE^i{}_ja^j\ .$$

It thus suffices to evaluate the operators Φ_1 and Φ_2.

To this end we find immediately that

$$\begin{aligned}\Phi_1=a_ia^i&=\tfrac{1}{2}[a_i,a^i]+\tfrac{1}{2}\{a_i,a^i\}\\ &=-(E^i{}_i-\delta^i{}_i)+\tfrac{1}{4}\{a_p,a^p\}\\ &=2n-I_1+\Delta\ ,\end{aligned} \tag{54}$$

where we have applied Eqs. (14) and (39), noting that $p=2$ for the case at hand, and $I_1=E^i{}_i$ is the first-order Gelfand invariant of U(n), corresponding to the total electron number operator. Similarly, for the operator Φ_2 a straightforward calculation, using Eq. (40), gives

$$\Phi_2=\Delta\Phi_1+2n^2+(2-n)I_1-I_2\ , \tag{55}$$

where $I_2=E^i{}_jE^j{}_i$ is the second-order Gelfand invariant of U(n). Substituting Eqs. (54) and (55) into Eq. (53) we thus obtain

$$\tau_r=(n-\bar{\epsilon}_{\bar{r}}-\Delta)(2n-I_1+\Delta)-2n^2-(2-n)I_1+I_2\ . \tag{56}$$

We now note that the eigenvalues of the U(n) invariant I_1 and I_2 are given, in terms of the U(n) Paldus labels $[a,b,c]$, by[8] [we use the same symbol for these eigenvalues since I_1 and I_2 are U(n) invariant]

$$\begin{aligned}&I_1=2a+b\ ,\\ &I_2=(2a+b)(n+1-a)+2a-(a+b)b\ .\end{aligned} \tag{57}$$

Also, in accordance with Eq. (12), the operator Δ may be written as

$$\Delta=\tilde{q}(2-\tilde{q})\ .$$

However, Eq. (42) indicates that Δ can only take values 0 and 1 so that, in particular, Δ is idempotent, i.e., $\Delta^2=\Delta$. It is easily checked, using Eq. (42), that the operator Δ may be alternatively expressed as

$$\Delta=\tfrac{1}{2}[1-(-1)^b]\ . \tag{58}$$

Substituting now Eqs. (57) and (58) into Eq. (56) we obtain, keeping in mind the idempotency of Δ, the following expression for the operators τ_r:

$$\tau_1=c(b+2-\Delta),\quad \tau_2=-(n+1-a)(b+\Delta)\ .$$

We also have [see Eq. (45)]

$$\xi_1=\bar{\epsilon}_1-\bar{\epsilon}_2=-\xi_2=1+b\ ,$$

so that substituting into Eq. (52) we obtain

$$\Gamma_1=\frac{c(b+2-\Delta)}{1+b},\quad \Gamma_2=\frac{(n+1-a)(b+\Delta)}{1+b}\ .$$

Substituting, finally, these expressions together with those of Eq. (49) into Eq. (50), we obtain the following formulas for the squared RME's R_r:

$$R_1=\frac{(n+2-c)(b+2-\Delta)}{b+2},\quad R_2=\frac{(a+1)(b+\Delta)}{b}\ . \tag{59}$$

We could similarly evaluate the squared RME's $\bar{R}_r$. However, in this case it suffices to use the relations[35]

$$\langle p-\delta_r||a||p\rangle=\left[\frac{D[p]}{D[p-\delta_r]}\right]^{1/2}\langle p||a||p-\delta_r\rangle\ ,$$

where[1,2,8]

$$D[p]=\frac{b+1}{n+1}\begin{bmatrix}n+1\\ a\end{bmatrix}\begin{bmatrix}n+1\\ c\end{bmatrix},\quad p=[a,b,c]$$

is the dimension of the irreducible representation $[a,b,c]$ of U(n). In this way we obtain the formulas

$$\bar{R}_1=\frac{(c+1)(b+\Delta)}{b},\quad \bar{R}_2=\frac{(n+2-a)(b+2-\Delta)}{b+2}\ , \tag{60}$$

where we have used the fact that for the final state $|p-\delta_r\rangle$ we have

$$\Delta'=\tfrac{1}{2}[1+(-1)^b]=1-\Delta\ .$$

We draw attention to the remarkable similarity between the squared RME's, Eqs. (59) and (60), and those obtained previously for the U($n+1$) generators in Ref. 8.

We are now ready to obtain explicit matrix representation for the O($2n+1$) generators. We first note that the O($2n+1$) Lie algebra is generated, as a Lie algebra, by the operators a^n and a_n together with the elementary U(n) generators $E^i{}_{i+1}$ and $E^{i+1}{}_i$ $(i=1,\ldots,n-1)$. Since the matrix elements of the latter operators are well known,[1,2,8] we only need to evaluate the matrix elements for the parafermion operators a^n and a_n. The matrix elements of the remaining O($2n+1$) generators may then be obtained by the repeated use of commutation relations.

Since the operators a^n and a_n do not alter the Paldus labels of the U($n-1$) subgroup, their nonzero matrix elements are [using notation of Eq. (46)]

$$W^r=\left\langle \begin{matrix} p_n+\delta_r \\ [P] \end{matrix} \middle| a^n \middle| \begin{matrix} p_n \\ [P] \end{matrix} \right\rangle ,$$
$$\overline{W}^r=\left\langle \begin{matrix} p_n-\delta_r \\ [P] \end{matrix} \middle| a_n \middle| \begin{matrix} p_n \\ [P] \end{matrix} \right\rangle . \tag{61}$$

In view of Eq. (47) we find that[8]

$$W^r=\left\langle \begin{matrix} p_n \\ [P] \end{matrix} \middle| R_r\overline{C}_r \middle| \begin{matrix} p_n \\ [P] \end{matrix} \right\rangle^{1/2} ,$$
$$\overline{W}^r=\left\langle \begin{matrix} p_n \\ [P] \end{matrix} \middle| \overline{R}_r C_r \middle| \begin{matrix} p_n \\ [P] \end{matrix} \right\rangle^{1/2} , \tag{62}$$

where the operators $\overline{C}_r, C_r$ are the U($n-1$) invariants given by

$$\overline{C}_r=\overline{P}[r]^n{}_n,\quad C_r=P[r]^n{}_n .$$

These operators may be expressed in terms of the U(n) and U($n-1$) Paldus labels $p_n=[a,b,c]$ and $p_{n-1}=[a',b',c']$, respectively, as follows:[8]

$$C_1=\frac{(\delta\overline{c})b}{(c+1)(b'+1)},\quad C_2=\frac{(\delta a)(b+2)}{(n+2-a)(b'+1)} ,$$
$$\overline{C}_1=\frac{(\delta c)(b+2)}{(n+2-c)(b'+1)},\quad \overline{C}_2=\frac{(\delta\overline{a})b}{(a+1)(b'+1)} , \tag{63}$$

where

$$\delta a=1-\delta\overline{a}=a-a' ,$$
$$\delta c=1-\delta\overline{c}=c-c' .$$

Substituting now Eqs. (59), (60), and (63) into Eq. (62) we obtain the desired elementary matrix elements

$$W^1=\overline{W}^2=\left[\frac{b+2-\Delta}{b'+1}\right]^{1/2},\quad W^2=\overline{W}^1=\left[\frac{b+\Delta}{b'+1}\right]^{1/2} . \tag{64}$$

We note that in the above formulas we have omitted the "selection factors" $\delta a, \delta c, \delta\overline{a}, \delta\overline{c}$ which can only take values 0 or 1 (cf., Ref. 8) and hence do not contribute to the structure of the matrix elements. It is therefore implicitly assumed that the matrix elements (61) vanish unless the Paldus labels of the final state are lexical.[1,2,8]

This essentially completes our discussion of the matrix elements of the second-order para-Fermi algebra. We note that it has been implicitly assumed that the phases of the matrix elements of the generators a^n and a_n are (+1), which is equivalent to the requirement that the RME's of Eqs. (46) and (48) have positive real phase. It is easily checked that this phase convention leads to the correct O($2n+1$) commutation relations as required.

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APPENDIX: O($2n+1$, 1) COMMUTATION RELATIONS

We demonstrate here that the operators (26) constitute the generators of an O($2n+1$, 1) group. Throughout this appendix we adopt the notation of Sec. III of the paper.

We start by defining the generators α_{RS} ($R,S=1,\ldots,2n+2$),

$$\alpha_{\rho\sigma}=\tfrac{1}{2}[a^\alpha{}_\rho, a^\alpha{}_\sigma] , \tag{A1a}$$

$$\alpha_{\rho,2n+1}=-\alpha_{2n+1,\rho}=a^\alpha{}_\rho/\sqrt{2} , \tag{A1b}$$

$$\alpha_{\rho,2n+2}=-\alpha_{2n+2,\rho}=i[\pi_\alpha, a^\alpha{}_\rho]/2\sqrt{2} , \tag{A1c}$$

$$\alpha_{2n+1,2n+2}=-\alpha_{2n+2,2n+1}=i\pi_\alpha/2 ,$$
$$\rho,\alpha=1,\ldots,2n \tag{A1d}$$

so that

$$\alpha_{RS}=-\alpha_{SR},\quad R,S=1,\ldots,2n+2 .$$

Note that these generators are identical with operators (26) except that $\pi_\alpha/2$ is replaced by $i\pi_\alpha/2$. It is our aim to show that the generators (A1) satisfy O($2n+2$) commutation relations,

$$[\alpha_{PQ},\alpha_{RS}]=g_{PS}\alpha_{QR}+g_{QR}\alpha_{PS}-g_{PR}\alpha_{QS}-g_{QS}\alpha_{PR} , \tag{A2}$$

where $g_{RS}=g_{SR}$ denotes the (symmetric) O($2n+2$) metric defined by

$$g_{\rho\sigma}=\begin{cases}1 & \text{if } |\rho-\sigma|=n \\ 0 & \text{otherwise,}\quad \rho,\sigma=1,\ldots,2n\end{cases}$$

$$g_{2n+1,2n+1}=g_{2n+2,2n+2}=-1 ,$$

$$g_{2n+1,2n+2}=g_{\rho,2n+1}=g_{\rho,2n+2}=0 .$$

In view of the well-known unitary trick of Weyl, the commutation relations, Eq. (A2), demonstrate that the operators (26) form the generators of the group O($2n+1$, 1) as required.

We know from the work of Bracken and Green[24] that the operators (A1a) and (A1b) satisfy the commutation relations of the group O($2n+1$) (cf. also Sec. I). It thus remains to demonstrate the commutation relations

$$[\alpha_{\rho\sigma},\alpha_{\mu,2n+2}]=g_{\mu\sigma}\alpha_{\rho,2n+2}-g_{\mu\rho}\alpha_{\sigma,2n+2} , \tag{A3a}$$

$$[\alpha_{2n+1,2n+2},\alpha_{\rho,2n+2}]=-\alpha_{\rho,2n+1} , \tag{A3b}$$

$$[\alpha_{\rho,2n+2},\alpha_{\sigma,2n+2}]=\alpha_{\rho\sigma} , \tag{A3c}$$

$$[\alpha_{\rho,2n+1},\alpha_{\sigma,2n+2}]=g_{\rho\sigma}\alpha_{2n+2,2n+1} , \tag{A3d}$$

the remaining ones being trivial.

We begin by recalling that $\{\pi_\alpha, a^\alpha{}_\rho\}=0$, ($\rho=1,\ldots,2n$), [cf. Eq. (25)], which yields, in particular, that

$$[\pi_\alpha, a^\alpha{}_\rho]=2\pi_\alpha a^\alpha{}_\rho \tag{A4}$$

and

$$[\pi_\alpha,[a^\alpha{}_\rho, a^\alpha{}_\sigma]]=0 . \tag{A5}$$

Using Eq. (A5) we thus get

$$\tfrac{1}{2}[[a^\alpha{}_\rho,a^\alpha{}_\sigma],[i\pi_\alpha,a^\alpha{}_\mu]]=\tfrac{1}{2}[i\pi_\alpha,[[a^\alpha{}_\rho,a^\alpha{}_\sigma],a^\alpha{}_\mu]]$$
$$=g_{\mu\sigma}i[\pi_\alpha,a^\alpha{}_\rho]-g_{\mu\rho}i[\pi_\alpha,a^\alpha{}_\sigma]\ ,$$

which is equivalent to the commutation relation (A3a).

We next prove the relation Eq. (A3b), which is equivalent to

$$[i\pi_\alpha/2,[i\pi_\alpha/2,a^\alpha{}_\rho]]=-a^\alpha{}_\rho\ .$$

Using Eq. (A4), we find

$$\begin{aligned}[i\pi_\alpha/2,[i\pi_\alpha/2,a^\alpha{}_\rho]]&=-\tfrac{1}{4}[\pi_\alpha,[\pi_\alpha,a^\alpha{}_\rho]]\\&=-\tfrac{1}{2}[\pi_\alpha,\pi_\alpha a^\alpha{}_\rho]\\&=-(\pi_\alpha/2)[\pi_\alpha,a^\alpha{}_\rho]\\&=-a^\alpha{}_\rho\ ,\end{aligned}\tag{A6}$$

as required, where in the last step we have used the result [cf. Eq. (25)]

$$\pi_\alpha{}^2=1\ .\tag{A7}$$

As to Eq. (A3c), we prove the equivalent relation

$$\tfrac{1}{4}[[\pi_\alpha,a^\alpha{}_\rho],[\pi_\alpha,a^\alpha{}_\sigma]]=[a^\alpha{}_\sigma,a^\alpha{}_\rho]\ .$$

Applying Eqs. (A4), (A6), and (A7) we find

$$\begin{aligned}\tfrac{1}{4}[[\pi_\alpha,a^\alpha{}_\rho],[\pi_\alpha,a^\alpha{}_\sigma]]&=[\pi_\alpha a^\alpha{}_\rho,\pi_\alpha a^\alpha{}_\sigma]\\&=-[a^\alpha{}_\sigma,a^\alpha{}_\rho]-\pi_\alpha[\pi_\alpha,a^\alpha{}_\rho]a^\alpha{}_\sigma\\&\quad+[\pi_\alpha,\pi_\alpha a^\alpha{}_\sigma]a^\alpha{}_\rho\\&=-[a^\alpha{}_\sigma,a^\alpha{}_\rho]-2a^\alpha{}_\rho a^\alpha{}_\sigma+2a^\alpha{}_\sigma a^\alpha{}_\rho\\&=[a^\alpha{}_\sigma,a^\alpha{}_\rho]\ ,\end{aligned}$$

as required.

It thus remains to establish Eq. (A3d) which is equivalent to the commutation relation

$$\tfrac{1}{2}[a^\alpha{}_\rho,[\pi_\alpha,a^\alpha{}_\sigma]]=-g_{\rho\sigma}\pi_\alpha\ .\tag{A8}$$

To this end we note that the left-hand side of Eq. (A8) may be written, in view of the anticommutation relations, Eqs. (23),

$$\begin{aligned}\tfrac{1}{2}[a^\alpha{}_\rho,[\pi_\alpha,a^\alpha{}_\sigma]]&=[a^\alpha{}_\rho,\pi_\alpha a^\alpha{}_\sigma]\\&=-\pi_\alpha\{a^\alpha{}_\rho,a^\alpha{}_\sigma\}\\&=-g_{\rho\sigma}\pi_\alpha\ ,\end{aligned}$$

as required. This proves the desired $O(2n+2)$ commutation relations, Eq. (A2).

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