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Complementarity relation between the U(p, q) and U(n) Lie groups and some applications to atomic physics

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Abstract. The complementarity relation between the unitary groups U(d) and U(n) within the symmetrical irreducible representations of the larger unitary group U(dn) is extended to non-compact groups. It is proved that the pseudo-unitary group U(p, q) is complementary with respect to U(n) within some positive discrete series irreducible representations of the larger pseudo-unitary group U(pn, qn). The latter arise when reducing the metaplectic irreducible representations $\langle(1/2)^{dn}\rangle$ and $\langle(1/2)^{dn-1}3/2\rangle$ of the real symplectic group Sp($2dn$, R), where $d=p+q$, and they are characterised by a single label, the eigenvalue of the first order Casimir operator. Some applications of the U(p, q)-U(n) complementarity to atomic physics are outlined. For such purposes, the isomorphism between the Lie algebras of SU(2, 2) and SO(4, 2) is used extensively. The mathematical framework underlying the Kibler-Négadi approach of the hydrogen atom dynamical group is extended to the independent-electron dynamical group of intrashell many-electron states, as well as to the correlated electron dynamical group of intrashell doubly excited states.

1. Introduction

In various physical applications of group theory, there occur direct product subgroups $G_1\times G_2$ of a larger group H, satisfying a special type of relation termed either complementarity (Moshinsky and Quesne 1970) or duality (Howe 1979, Gelbart 1979). Following Moshinsky and Quesne (1970), the subgroups G_1 and G_2 are referred to as complementary within a definite irreducible representation (irrep) μ of H if the irreps $\lambda_1\times\lambda_2$ of $G_1\times G_2$ contained in μ are multiplicity free, and there is a one-to-one correspondence between the labels of such associated irreps λ_1 and λ_2.

A well known example of complementary Lie groups is provided by the pair of unitary groups U(d) and U(n) once one considers either symmetrical or antisymmetrical irreps of the larger unitary group U(dn), characterised by one-row $\{\rho\}$ or one-column $\{1^\rho\}$ Young diagrams respectively (Baird and Biedenharn 1963, Moshinsky 1963, 1968). The symmetrical irreps $\{\rho\}$ (respectively the antisymmetrical irreps $\{1^\rho\}$) of U(dn) indeed decompose under U(d)$\times$U(n) into a direct sum of irreps $\{h\}\times\{h\}$, where $\{h\}=\{h_1,\ldots,h_m\}$ runs over all the partitions of ρ into $m=\min(d,n)$ integers (respectively a direct sum of irreps $\{h\}\times\{\tilde{h}\}$, where $\{h\}=\{h_1,\ldots,h_d\}$ runs over all the partitions of ρ into d integers not exceeding n and $\{\tilde{h}\}$ is the partition conjugate to $\{h\}$). Other examples of complementary Lie groups can be found in recent publications (Quesne 1985a, b).

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The aim of the present paper is to extend to non-compact groups the above-mentioned complementarity between U(d) and U(n) within the symmetrical irreps $\{\rho\}$ of U(dn). Setting $d=p+q$, we shall demonstrate that the pseudo-unitary group U(p, q) is complementary with respect to U(n) within some positive discrete series irreps of U(pn, qn). As the symmetrical irreps of U(dn), such irreps of U(pn, qn) are characterised by a single label ρ.

Two special cases of the U(p, q)-U(n) complementarity have already been reported in the physical literature: the case where $p=q=n=3$ by Flores (1967), who did not, however, completely identify the U(3, 3) group, and the one where $p=q$, $n=1$ by Couvreur *et al* (1983). As far as the general case is considered, this has been discussed in the mathematical literature (Gross and Kunze 1977, Kashiwara and Vergne 1978, Gelbart 1979), but we feel the need to update this discussion to the field of physics and to demonstrate its usefulness in specific applications as reviewed at the end of the present paper†. Other applications to SU(n) representation theory will be dealt with in forthcoming publications.

In § 2, by starting with a boson realisation of the symplectic group Sp($2dn, R$), where $d=p+q$, we introduce a U(pn, qn) subgroup of the latter and show that the irreps of such a subgroup are positive discrete series specified by a single integer ρ. In § 3, we define U(p, q) and U(n) subgroups of U(pn, qn), characterise their irreps contained in a given irrep of U(pn, qn) and state their complementarity relation. In §§ 4 and 5, we prove the latter in the cases where $n \geqslant p+q$ and $n<p+q$ respectively. Finally, in § 6, we outline some applications to atomic physics.

2. The U(pn, qn) subgroup of Sp($2dn, R$), where $d=p+q$, and its irreducible representations

As is well known (Moshinsky and Quesne 1971), the Sp($2dn, R$) generators can be realised in terms of dn boson creation operators η_{is}, $i=1,\ldots,d$, $s=1,\ldots,n$ and the corresponding annihilation operators ξ_{is} as follows:

$$\begin{aligned}
&\mathbb{D}^{\dagger}_{is,jt}=\mathbb{D}^{\dagger}_{jt,is}=\eta_{is}\eta_{jt} && (is)\leqslant(jt)\\
&\mathbb{D}_{is,jt}=\mathbb{D}_{jt,is}=\xi_{is}\xi_{jt} && (is)\leqslant(jt)\\
&\mathbb{E}_{is,jt}=\tfrac{1}{2}(\eta_{is}\xi_{jt}+\xi_{jt}\eta_{is})=\eta_{is}\xi_{jt}+\tfrac{1}{2}\delta_{ij}\delta_{st}
\end{aligned}\tag{2.1}$$

where $i, j=1,\ldots,d$ and $s, t=1,\ldots,n$. Their commutation relations are given by

$$\begin{aligned}
&[\mathbb{E}_{is,jt},\mathbb{E}_{i's',j't'}]=\delta_{ji'}\delta_{ts'}\mathbb{E}_{is,j't'}-\delta_{ij'}\delta_{st'}\mathbb{E}_{i's',jt}\\
&[\mathbb{E}_{is,jt},\mathbb{D}^{\dagger}_{i's',j't'}]=\delta_{ji'}\delta_{ts'}\mathbb{D}^{\dagger}_{is,j't'}+\delta_{jj'}\delta_{tt'}\mathbb{D}^{\dagger}_{is,i's'}\\
&[\mathbb{E}_{is,jt},\mathbb{D}_{i's',j't'}]=-\delta_{ii'}\delta_{ss'}\mathbb{D}_{jt,j't'}-\delta_{ij'}\delta_{st'}\mathbb{D}_{jt,i's'}\\
&[\mathbb{D}^{\dagger}_{is,jt},\mathbb{D}^{\dagger}_{i's',j't'}]=[\mathbb{D}_{is,jt},\mathbb{D}_{i's',j't'}]=0\\
&[\mathbb{D}_{is,jt},\mathbb{D}^{\dagger}_{i's',j't'}]=\delta_{ii'}\delta_{ss'}\mathbb{E}_{j't',jt}+\delta_{ij'}\delta_{st'}\mathbb{E}_{i's',jt}+\delta_{ji'}\delta_{ts'}\mathbb{E}_{j't',is}+\delta_{jj'}\delta_{tt'}\mathbb{E}_{i's',is}.
\end{aligned}\tag{2.2}$$

In addition, they satisfy the following Hermiticity properties:

$$\mathbb{D}_{is,jt}=(\mathbb{D}^{\dagger}_{is,jt})^{\dagger}\qquad \mathbb{E}_{is,jt}=(\mathbb{E}_{jt,is})^{\dagger}.\tag{2.3}$$

† After completion of the present work, King and Wybourne (1985) published a paper, wherein the chain U(pn, qn) ⊃ U(p, q) × U(n) is used to derive branching rules from U(p, q) to U(p) × U(q) by the Schur function technique.

In the realisation (2.1), the Sp($2dn$, R) group has only two (metaplectic) irreps. They are positive discrete series irreps, characterised by their lowest weight $\langle (1/2)^{dn}\rangle$ or $\langle (1/2)^{dn-1}3/2\rangle$, and their carrier space is the set of boson states with an even or odd boson number respectively.

Let us set $d=p+q$, where without loss of generality we may assume $p\geqslant q$, and let us define the operators $\mathbb{P}_{is,jt}$, $i,j=1,\ldots,d$, s, $t=1,\ldots,n$ by the following relations:

$$\begin{aligned}
\mathbb{P}_{is,jt} &= \mathbb{E}_{is,jt} && \text{if } i,j=1,\ldots,p && (2.4a)\\
&= \mathbb{E}_{jt,is} && \text{if } i,j=p+1,\ldots,d && (2.4b)\\
&= \mathbb{D}^{\dagger}_{is,jt} && \text{if } i=1,\ldots,p \text{ and } j=p+1,\ldots,d && (2.4c)\\
&= \mathbb{D}_{is,jt} && \text{if } i=p+1,\ldots,d \text{ and } j=1,\ldots,p. && (2.4d)
\end{aligned}$$

From the commutation relations and Hermiticity properties of the Sp($2dn$, R) generators, those of the operators $\mathbb{P}_{is,jt}$ are, respectively, obtained as

$$[\mathbb{P}_{is,jt},\mathbb{P}_{i's',j't'}]=g_{jt,i's'}\mathbb{P}_{is,j't'}-g_{j't',is}\mathbb{P}_{i's',jt} \qquad (2.5)$$

and

$$\mathbb{P}_{is,jt}=(\mathbb{P}_{jt,is})^{\dagger} \qquad (2.6)$$

where the metric tensor $g_{is,jt}$ is defined by

$$g_{is,jt}=\varepsilon_i\delta_{ij}\delta_{st} \qquad (2.7)$$

and

$$\left.\begin{aligned}
\varepsilon_i &= 1 && \text{if } i=1,\ldots,p\\
&= -1 && \text{if } i=p+1,\ldots,d.
\end{aligned}\right\} \qquad (2.8)$$

The operators $\mathbb{P}_{is,jt}$ are therefore the generators of a U(pn, qn) subgroup of Sp($2dn$, R). The maximal compact subgroup of U(pn, qn) is the direct product group U(pn)$\times$ U(qn), whose factors are generated by the operators (2.4a) and (2.4b) respectively.

From equation (2.5), the weight generators of U(pn, qn) are the operators $\mathbb{P}_{is,is}=\mathbb{E}_{is,is}$, $i=1,\ldots,d$, $s=1,\ldots,n$. Let us enumerate the values of the double index is in lexical order: $11,\ldots,1n,21,\ldots,2n,\ldots,d1,\ldots,dn$. The lowering generators are those operators $\mathbb{P}_{is,jt}$ for which either $(is)>(jt)$, $i,j=1,\ldots,p$, s, $t=1,\ldots,n$ or $(is)<(jt)$, $i,j=p+1,\ldots,d$, s, $t=1,\ldots,n$ or $i=p+1,\ldots,d$, $j=1,\ldots,p$, s, $t=1,\ldots,n$.

The U(pn, qn) irreps to be dealt with in the present problem are positive discrete series irreps characterised by their lowest weight $\{f_{pn}+\frac12,\ldots,f_{11}+\frac12; f'_{qn}+\frac12,\ldots,f'_{11}+\frac12\}$, where $\{f_{11},\ldots,f_{pn}\}$ and $\{f'_{11},\ldots,f'_{qn}\}$ are two partitions. The lowest weight state $|\mathrm{LWS}\rangle$ of such irreps satisfies the following system of equations:

$$\begin{aligned}
\mathbb{P}_{is,is}|\mathrm{LWS}\rangle &= (f_{p+1-i,n+1-s}+\tfrac12)|\mathrm{LWS}\rangle && i=1,\ldots,p\\
&= (f'_{d+1-i,n+1-s}+\tfrac12)|\mathrm{LWS}\rangle && i=p+1,\ldots,d\\
\mathbb{P}_{is,jt}|\mathrm{LWS}\rangle &= 0 \qquad (is)>(jt) && i,j=1,\ldots,p \qquad (2.9)\\
&= 0 \qquad (is)<(jt) && i,j=p+1,\ldots,d\\
&= 0 \qquad i=p+1,\ldots,d && j=1,\ldots,p
\end{aligned}$$

where $s,t=1,\ldots,n$. It is the lowest weight state of an irrep $\{f_{11}+\frac12,\ldots,f_{pn}+\frac12\}\times\{f'_{11}+\frac12,\ldots,f'_{qn}+\frac12\}$ of the maximal compact subgroup U(pn)$\times$U(qn).

By extending to arbitrary values of p, q and n the work of Couvreur *et al* (1983) for $p=q$ and $n=1$, it is easy to show that for the realisation (2.4) of the U(pn, qn) generators, equation (2.9) only has a solution in either one of the three following cases: (i) $f_{11}=\rho>0$, $f_{12}=\ldots=f_{pn}=f'_{11}=\ldots=f'_{qn}=0$; (ii) $f'_{11}=-\rho>0$, $f_{11}=\ldots=f_{pn}=f'_{12}=\ldots=f'_{qn}=0$ and (iii) $f_{11}=\ldots=f_{pn}=f'_{11}=\ldots=f'_{qn}=\rho=0$. This solution is

$$\begin{aligned} |\text{LWS}\rangle &= (\eta_{pn})^{\rho}|0\rangle && \text{in case (i)} \\ &= (\eta_{dn})^{-\rho}|0\rangle && \text{in case (ii)} \\ &= |0\rangle && \text{in case (iii)} \end{aligned} \tag{2.10}$$

where $|0\rangle$ is the boson vacuum state. The U(pn, qn) irreps contained in either irrep $\langle(1/2)^{dn}\rangle$ or $\langle(1/2)^{dn-1}3/2\rangle$ of Sp($2dn$, R) can be denoted by the shorthand notation $[\rho]$, $\rho\in \boldsymbol{Z}$, defined as follows:

$$\begin{aligned} [\rho] &= \{(1/2)^{pn-1}, \rho+\tfrac{1}{2}; (1/2)^{qn}\} && \text{if } \rho>0 \\ &= \{(1/2)^{pn}; (1/2)^{qn-1}, -\rho+\tfrac{1}{2}\} && \text{if } \rho<0 \\ &= \{(1/2)^{pn}; (1/2)^{qn}\} && \text{if } \rho=0. \end{aligned} \tag{2.11}$$

The branching rules can be written as

$$\langle(1/2)^{dn}\rangle \downarrow \sum_{\substack{\rho=-\infty \\ \rho\ \text{even}}}^{+\infty} \oplus[\rho]$$

and

$$\langle(1/2)^{dn-1}3/2\rangle \downarrow \sum_{\substack{\rho=-\infty \\ \rho\ \text{odd}}}^{+\infty} \oplus[\rho]. \tag{2.12}$$

The label ρ specifying the U(pn, qn) irreps in equations (2.11) and (2.12) has a very simple meaning. Let us indeed consider the U(pn, qn) first order Casimir operator

$$\mathbb{G}_1=\sum_{is} \varepsilon_i \mathbb{P}_{is,is}. \tag{2.13}$$

By applying it to the lowest weight state (2.10), we obtain the equation

$$\mathbb{G}_1|\text{LWS}\rangle=[\rho+\tfrac{1}{2}(p-q)n]|\text{LWS}\rangle \tag{2.14}$$

valid in all three cases $\rho>0$, $\rho<0$ and $\rho=0$. Apart from an irrelevant constant, ρ is therefore the eigenvalue of the first order Casimir operator $\mathbb{G}_1$ of U(pn, qn). Let us note that ρ has a similar meaning for the symmetrical irreps $\{\rho\}$ of the compact group U(dn). The irreps (2.11) of U(pn, qn) may therefore be considered as the infinite-dimensional counterpart for pseudo-unitary groups of the U(dn) finite-dimensional irreps $\{\rho\}$.

3. The U(p, q) × U(n) subgroup of U(pn, qn) and its irreducible representations

By contracting the U(pn, qn) generators with respect to index i or s, we obtain the operators

$$P_{ij}=\sum_{s} \mathbb{P}_{is,js} \qquad i,j=1,\ldots,d \tag{3.1}$$

and

$$\mathcal{P}_{st} = \sum_i \varepsilon_i \mathbb{P}_{is,it} \qquad s, t = 1, \ldots, n. \tag{3.2}$$

From equations (2.5) and (2.6), it follows that the operators P_{ij} satisfy the following commutation relations and Hermiticity properties:

$$[P_{ij}, P_{i'j'}] = g_{ji'} P_{ij'} - g_{j'i} P_{i'j} \tag{3.3}$$

$$P_{ij} = (P_{ji})^\dagger \tag{3.4}$$

where

$$g_{ij} = \varepsilon_i \delta_{ij}. \tag{3.5}$$

Hence they generate a $U(p, q)$ subgroup of $U(pn, qn)$. The corresponding relations for the operators $\mathcal{P}_{st}$ are

$$[\mathcal{P}_{st}, \mathcal{P}_{s't'}] = \delta_{ts'} \mathcal{P}_{st'} - \delta_{t's} \mathcal{P}_{s't} \tag{3.6}$$

and

$$\mathcal{P}_{st} = (\mathcal{P}_{ts})^\dagger \tag{3.7}$$

showing that such operators generate a $U(n)$ subgroup of $U(pn, qn)$. Since

$$[P_{ij}, \mathcal{P}_{st}] = 0 \tag{3.8}$$

the $U(pn, qn)$ group actually contains the direct product subgroup $U(p, q) \times U(n)$. We therefore obtain the following group chain

$$\mathrm{Sp}(2dn, R) \supset U(pn, qn) \supset U(p, q) \times U(n) \qquad d = p + q. \tag{3.9}$$

At this point, it is worth noting that $U(p, q)$ also belongs to the group chain

$$\mathrm{Sp}(2dn, R) \supset \mathrm{Sp}(2d, R) \supset U(p, q) \qquad d = p + q \tag{3.10}$$

where $\mathrm{Sp}(2d, R)$ is generated by the operators

$$D^+_{ij} = \sum_s \mathbb{D}^+_{is,js} \qquad D_{ij} = \sum_s \mathbb{D}_{is,js} \qquad E_{ij} = \sum_s \mathbb{E}_{is,js}. \tag{3.11}$$

From equations (2.4) and (3.1), the $U(p, q)$ generators can indeed be expressed in terms of the $\mathrm{Sp}(2d, R)$ ones as follows:

$$\begin{aligned} P_{ij} &= E_{ij} && \text{if } i, j = 1, \ldots, p \\ &= E_{ji} && \text{if } i, j = p+1, \ldots, d \\ &= D^+_{ij} && \text{if } i = 1, \ldots, p \text{ and } j = p+1, \ldots, d \\ &= D_{ij} && \text{if } i = p+1, \ldots, d \text{ and } j = 1, \ldots, p. \end{aligned} \tag{3.12}$$

The weight and lowering generators of $U(p, q)$ are the operators

$$P_{ii} = E_{ii} = \sum_s \eta_{is} \xi_{is} + \tfrac{1}{2} n \qquad i = 1, \ldots, d \tag{3.13}$$

and

$$\begin{aligned} P_{ij} &= E_{ij} = \sum_s \eta_{is} \xi_{js} && 1 \leqslant j < i \leqslant p \\ &= E_{ji} = \sum_s \eta_{js} \xi_{is} && p+1 \leqslant i < j \leqslant d \\ &= D_{ij} = \sum_s \xi_{is} \xi_{js} && i = p+1, \ldots, d \qquad j = 1, \ldots, p \end{aligned} \tag{3.14}$$

respectively, whereas the weight and raising generators of U(n) are given by

$$\mathscr{P}_{ss}=\sum_i{}' \eta_{is}\xi_{is}-\sum_i{}'' \eta_{is}\xi_{is}+\tfrac{1}{2}(p-q) \qquad s=1,\ldots,n \tag{3.15}$$

and

$$\mathscr{P}_{st}=\sum_i{}' \eta_{is}\xi_{jt}-\sum_i{}'' \eta_{it}\xi_{js} \qquad 1\leqslant s<t\leqslant n \tag{3.16}$$

respectively. In equations (3.15) and (3.16), prime and double prime summations are defined by

$$\sum_i{}'=\sum_{i=1}^{p} \qquad \sum_i{}''=\sum_{i=p+1}^{d}. \tag{3.17}$$

It remains to determine the branching rule for the irreps $[\rho]$ of U(pn, qn) under U(pn, qn)$\downarrow$U(p, q)$\times$U(n). The U(n) irreps are characterised by their highest weight $\{j_1+(p-q)/2, j_2+(p-q)/2,\ldots,j_n+(p-q)/2\}$, where $j_1, j_2,\ldots,j_n$ are some integers satisfying the inequalities $j_1\geqslant\ldots\geqslant j_n$. From the definition (3.15) of the U(n) weight generators, we note that $j_1,\ldots,j_n$ may assume negative as well as non-negative values and hence correspond to mixed irreps of U(n) (Flores 1967, Flores and Moshinsky 1967, King 1970, 1975). We shall henceforth denote the U(n) irreps by the shorthand notation

$$[j_1j_2\ldots j_n]=\{j_1+(p-q)/2, j_2+(p-q)/2,\ldots,j_n+(p-q)/2\}. \tag{3.18}$$

The U(p, q) irreps contained in a positive discrete series irrep $[\rho]$ of U(pn, qn) are also positive discrete series irreps characterised by their lowest weight $\{k_p+n/2,\ldots,k_2+n/2,\ k_1+n/2;\ k'_q+n/2,\ldots,k'_2+n/2,\ k'_1+n/2\}$, where $\{k_1k_2\ldots k_p\}$ and $\{k'_1k'_2\ldots k'_q\}$ are two partitions. We shall denote such irreps by the shorthand notation

$$[k_1k_2\ldots k_p;\ k'_1k'_2\ldots k'_q]$$
$$=\{k_p+n/2,\ldots,k_2+n/2,\ k_1+n/2;\ k'_q+n/2,\ldots,k'_2+n/2,\ k'_1+n/2\}. \tag{3.19}$$

Let us now state the main result of the present paper: the U(p, q) and U(n) groups are complementary within any irrep $[\rho]$ of U(pn, qn) or, in other words, the irreps $[k_1\ldots k_p;\ k'_1\ldots k'_q]\times[j_1\ldots j_n]$ of U(p, q)$\times$U(n), contained in a given irrep $[\rho]$ of U(pn, qn), are multiplicity free and there is a one-to-one correspondence between the labels $j_1,\ldots,j_n$ of the U(n) irreps and the labels $k_1,\ldots,k_p, k'_1,\ldots,k'_q$ of the associated U(p, q) irreps. The precise relation between both sets of labels depends on the relative values of p, q and n and is given in table 1. In particular, the labels satisfy the condition

$$\sum_\alpha k_\alpha-\sum_\beta k'_\beta=\sum_s j_s=\rho \tag{3.20}$$

Table 1. U(p, q)$\times$U(n) irreps contained in a given irrep $[\rho]$ of U(pn, qn).

n	$[k_1\ldots k_p;\ k'_1\ldots k'_q]$	$[j_1\ldots j_n]$	σ
$n\geqslant p+q$	$[k_1\ldots k_p;\ k'_1\ldots k'_q]$	$[k_1\ldots k_p0^{n-p-q}-k'_q\ldots-k'_1]$	—
$p\leqslant n<p+q$	$[k_1\ldots k_{n-q+\sigma}0^{p+q-n-\sigma};\ k'_1\ldots k'_{q-\sigma}0^\sigma]$	$[k_1\ldots k_{n-q+\sigma}-k'_{q-\sigma}\ldots-k'_1]$	$0,1,\ldots,p+q-n$
$q\leqslant n<p$	$[k_1\ldots k_{n-q+\sigma}0^{p+q-n-\sigma};\ k'_1\ldots k'_{q-\sigma}0^\sigma]$	$[k_1\ldots k_{n-q+\sigma}-k'_{q-\sigma}\ldots-k'_1]$	$0,1,\ldots,q$
$n<q$	$[k_1\ldots k_\sigma0^{p-\sigma};\ k'_1\ldots k'_{n-\sigma}0^{q-n+\sigma}]$	$[k_1\ldots k_\sigma-k'_{n-\sigma}\ldots-k'_1]$	$0,1,\ldots,n$

where the indices α and β run from 1 to p and from 1 to q respectively. Equation (3.20) results from the equality

$$G_1 = \mathscr{G}_1 = \mathbb{G}_1 \tag{3.21}$$

where G_1 and $\mathscr{G}_1$ are the first order Casimir operators of $\mathrm{U}(p, q)$ and $\mathrm{U}(n)$, defined by

$$G_1 = \sum_i \varepsilon_i P_{ii} \qquad \mathscr{G}_1 = \sum_s \mathscr{P}_{ss} \tag{3.22}$$

respectively.

The proof of the $\mathrm{U}(p, q)$-$\mathrm{U}(n)$ complementarity is detailed in the next two sections. It consists in determining all the states $|\ \rangle$ satisfying the following two conditions: (i) to be the lowest weight state of some $\mathrm{U}(p, q)$ irrep $[k_1 \ldots k_p; k'_1 \ldots k'_q]$ and (ii) to be the highest weight state of some $\mathrm{U}(n)$ irrep $[j_1 \ldots j_n]$. Such states are the simultaneous solutions of the following system of equations:

$$(E_{ii} - \tfrac{1}{2}n)|\ \rangle = \sum_s \eta_{is}\xi_{is}|\ \rangle = \begin{cases} k_{p+1-i}|\ \rangle & i = 1, \ldots, p \\ k'_{d+1-i}|\ \rangle & i = p+1, \ldots, d \end{cases} \tag{3.23a}$$

$$E_{ij}|\ \rangle = \sum_s \eta_{is}\xi_{js}|\ \rangle = 0 \qquad 1 \leqslant j < i \leqslant p, p+1 \leqslant j < i \leqslant d \tag{3.23b}$$

$$D_{ij}|\ \rangle = \sum_s \xi_{is}\xi_{js}|\ \rangle = 0 \qquad i = 1, \ldots, p, j = p+1, \ldots, d \tag{3.23c}$$

$$[\mathscr{P}_{ss} - \tfrac{1}{2}(p-q)]|\ \rangle = \left(\sum_i{}' \eta_{is}\xi_{is} - \sum_i{}'' \eta_{is}\xi_{is}\right)|\ \rangle = j_s|\ \rangle \qquad s = 1, \ldots, n \tag{3.23d}$$

$$\mathscr{P}_{st}|\ \rangle = \left(\sum_i{}' \eta_{is}\xi_{it} - \sum_i{}'' \eta_{it}\xi_{is}\right)|\ \rangle = 0 \qquad 1 \leqslant s < t \leqslant n. \tag{3.23e}$$

It will be shown that this system has a solution if and only if the labels of the $\mathrm{U}(p, q)$ and $\mathrm{U}(n)$ irreps are related as shown in table 1 and that such a solution is unique.

4. Proof of the complementarity relation when $n \geqslant p+q$

In solving equation (3.23), we have to distinguish between the following four cases: $n \geqslant p+q$, $p \leqslant n < p+q$, $q \leqslant n < p$ and $n < q$. We shall start with the first one, which is the simplest, and leave the three remaining ones for the next section.

Equations (3.23a) and (3.23b) are the conditions to be satisfied by the lowest weight state of a $\mathrm{U}(p) \times \mathrm{U}(q)$ irrep characterised by $\{k_1 \ldots k_p\} \times \{k'_1 \ldots k'_q\}$. All their solutions can be written as (Moshinsky 1962)

$$|\ \rangle = \prod_{\alpha=1}^{p} (\eta_{p-\alpha+1\ldots p,1\ldots\alpha})^{k_\alpha - k_{\alpha+1}} (\eta_{d-\beta+1\ldots d,n-\beta+1\ldots n})^{k'_\beta - k'_{\beta+1}}$$
$$\times Z\left(\frac{\eta_{ps}}{\eta_{p1}}, \frac{\eta_{p-1p,1s}}{\eta_{p-1p,12}}, \ldots, \frac{\eta_{1\ldots p,1\ldots p-1s}}{\eta_{1\ldots p,1\ldots p}}, \frac{\eta_{ds}}{\eta_{dn}}, \frac{\eta_{d-1d,sn}}{\eta_{d-1d,n-1n}}, \ldots, \frac{\eta_{p+1\ldots d,sn-q+2\ldots n}}{\eta_{p+1\ldots d,n-q+1\ldots n}}\right). \tag{4.1}$$

In equation (4.1), k_{p+1} and k'_{q+1} are assumed to vanish, the operators $\eta_{p-\alpha+1\ldots p,1\ldots\alpha-1s}$, $\alpha = 1, \ldots, p$, $s = \alpha, \ldots, n$ are defined by

$$\eta_{p-\alpha+1\ldots p,1\ldots\alpha-1s} = \sum_\pi (-1)^\pi \eta_{p-\alpha+1,\pi(1)} \cdots \eta_{p-1,\pi(\alpha-1)}\eta_{p,\pi(s)} \tag{4.2}$$

where the summation is carried out over the $\alpha!$ permutations of the indices $1, \ldots, \alpha-1$, s; the operators $\eta_{d-\beta+1\ldots d, sn-\beta+2\ldots n}$, $\beta=1, \ldots, q$, $s=1, \ldots, n-\beta+1$ are defined by a similar relation, and Z is an arbitrary polynomial in the indicated variables, subject to the condition that, when multiplied by the other factors in (4.1), it should still be a polynomial in η_{is}.

Next let us solve equation (3.23e). Here, it is convenient to replace in Z the pq ratios $\eta_{p-\alpha+1\ldots p,1\ldots\alpha-1n-\beta+1}/\eta_{p-\alpha+1\ldots p,1\ldots\alpha}$, $\alpha=1, \ldots, p$, $\beta=1, \ldots, q$ by

$$x_{\alpha\beta}/(\eta_{p-\alpha+1\ldots p,1\ldots\alpha}\eta_{d-\beta+1\ldots d,n-\beta+1\ldots n}) \qquad \alpha=1, \ldots p \qquad \beta=1, \ldots, q \tag{4.3}$$

where the operators $x_{\alpha\beta}$, defined by

$$x_{\alpha\beta}=\sum_s \eta_{p-\alpha+1\ldots p,1\ldots\alpha-1s}\eta_{d-\beta+1\ldots d,sn-\beta+2\ldots n} \qquad \alpha=1, \ldots, p \qquad \beta=1, \ldots, q \tag{4.4}$$

satisfy the relations

$$[\mathscr{P}_{st}, x_{\alpha\beta}]=0 \qquad 1\leqslant s<t\leqslant n. \tag{4.5}$$

After such a substitution, Z becomes a new polynomial Z' in the ratios (4.3) and the following ratios:

$$\begin{aligned} &\eta_{p-\alpha+1\ldots p,1\ldots\alpha-1s}/\eta_{p-\alpha+1\ldots p,1\ldots\alpha} && \alpha=1, \ldots, p && s=\alpha+1, \ldots, n-q \\ &\eta_{d-\beta+1\ldots d,sn-\beta+2\ldots n}/\eta_{d-\beta+1\ldots d,n-\beta+1\ldots n} && \beta=1, \ldots, q && s=1, \ldots, n-\beta. \end{aligned} \tag{4.6}$$

It is then straightforward to show that equation (3.23e) imposes that Z' only depends on the ratios (4.3). By expanding Z' into a power series, we obtain the following expression for the simultaneous solutions of equations (3.23a), (3.23b) and (3.23e):

$$\begin{aligned} |\;\rangle = \sum_{\{\lambda_{\alpha\beta}\}} C_{\{\lambda_{\alpha\beta}\}}\left(\prod_{\alpha=1}^{p}(\eta_{p-\alpha+1\ldots p,1\ldots\alpha})^{k_\alpha-k_{\alpha+1}-\Sigma_\beta\lambda_{\alpha\beta}}\right) \\ \times\left(\prod_{\beta=1}^{q}(\eta_{d-\beta+1\ldots d,n-\beta+1\ldots n})^{k'_\beta-k'_{\beta+1}-\Sigma_\alpha\lambda_{\alpha\beta}}\right)\left(\prod_{\alpha=1}^{p}\prod_{\beta=1}^{q}(x_{\alpha\beta})^{\lambda_{\alpha\beta}}\right)|0\rangle. \end{aligned} \tag{4.7}$$

Here $C_{\{\lambda_{\alpha\beta}\}}$ is an, as yet, undetermined constant and the summation indices $\lambda_{\alpha\beta}$, $\alpha=1, \ldots, p$, $\beta=1, \ldots, q$ are restricted by the condition that the right-hand side of equation (4.7) should be a polynomial in η_{is}.

Equation (3.23d) now yields the following conditions:

$$\begin{aligned} &\sum_\beta \lambda_{s\beta}=k_s-j_s && s=1, \ldots, p \\ &\sum_\alpha \lambda_{\alpha,n-s+1}=k'_{n-s+1}+j_s && s=n-q+1, \ldots, n \end{aligned} \tag{4.8}$$

and

$$j_s=0 \qquad s=p+1, \ldots, n-q. \tag{4.9}$$

From equation (3.20), equation (4.8) contains only $p+q-1$ independent relations, which would enable us to express $p+q-1$ indices $\lambda_{\alpha\beta}$ in terms of the remaining ones. We shall, however, not need to find a detailed solution of equation (4.8), since we shall show hereafter that all the $\lambda_{\alpha\beta}$ indices must actually vanish. For the time being, it is enough to introduce equation (4.8) into equation (4.7), which now reads

$$| \rangle = \left(\prod_{\alpha=1}^{p} (\eta_{p-\alpha+1\ldots p,1\ldots\alpha})^{j_\alpha - k_{\alpha+1}} \right) \times \left(\prod_{\beta=1}^{q} (\eta_{d-\beta+1\ldots d,n-\beta+1\ldots n})^{-j_{n-\beta+1} - k'_{\beta+1}} \right) \times \left(\sum_{\{\lambda_{\alpha\beta}\}} C_{\{\lambda_{\alpha\beta}\}} \prod_{\alpha=1}^{p} \prod_{\beta=1}^{q} (x_{\alpha\beta})^{\lambda_{\alpha\beta}} \right) |0\rangle. \tag{4.10}$$

To solve the last equation (3.23c), it is convenient to extend the concept of traceless boson operators introduced by Lohe and Hurst (1971) to construct bases for $O(n)$ and $USp(n)$ irreps. In the present context, traceless boson operators are introduced in the following way. Let $P(\eta_{11}, \ldots, \eta_{dn})|0\rangle$ be any boson state satisfying the conditions

$$\sum_s \xi_{is}\xi_{js} P(\eta_{11}, \ldots, \eta_{dn})|0\rangle = 0 \qquad i = 1, \ldots, p \qquad j = p+1, \ldots, d. \tag{4.11}$$

Let us look for some modified boson operators $a^\dagger_{is}$ and a_{is}, $i = 1, \ldots, d$, $s = 1, \ldots, n$ such that the transformed states under the action of $a^\dagger_{is}$ or a_{is} still fulfil the same conditions, i.e.

$$\left(\sum_s \xi_{is}\xi_{js} \right) a^\dagger_{kt} P(\eta_{11}, \ldots, \eta_{dn})|0\rangle = \left(\sum_s \xi_{is}\xi_{js} \right) a_{kt} P(\eta_{11}, \ldots, \eta_{dn})|0\rangle = 0$$
$$i = 1, \ldots, p, j = p+1, \ldots, d, k = 1, \ldots, d, t = 1, \ldots, n. \tag{4.12}$$

For the annihilation operators a_{is}, we may take the standard boson annihilation operators:

$$a_{is} = \xi_{is} \qquad i = 1, \ldots, d \qquad s = 1, \ldots, n. \tag{4.13}$$

On the contrary, the creation operators $a^\dagger_{is}$ differ from η_{is} and may be written as

$$a^\dagger_{is} = \begin{cases} \eta_{is} - \sum'_{j} \sum''_{kl} \left(\sum_t \eta_{jt}\eta_{kt} \right) \Delta^{-1}_{jk,il} \xi_{ls} & i = 1, \ldots, p \qquad s = 1, \ldots, n \\ \eta_{is} - \sum'_{jl} \sum''_{k} \left(\sum_t \eta_{jt}\eta_{kt} \right) \Delta^{-1}_{jk,li} \xi_{ls} & i = p+1, \ldots, d \qquad s = 1, \ldots, n \end{cases} \tag{4.14}$$

where $\boldsymbol{\Delta}$ is a $pq \times pq$ operator matrix, whose elements are defined by

$$\Delta_{ij,kl} = \delta_{ik} E_{lj} + \delta_{jl} E_{ki} \qquad i, k = 1, \ldots, p \qquad j, l = p+1, \ldots, d \tag{4.15}$$

and $\boldsymbol{\Delta}^{-1}$ is its inverse. Various properties of the operators $a^\dagger_{is}$ and a_{is} are listed in appendix 1. In particular, it is proved there that if we replace η_{is} by $a^\dagger_{is}$ in equation (4.10), the resulting states are still solutions of equations (3.23a), (3.23b), (3.23d) and (3.23e), and in addition satisfy equation (3.23c).

It now only remains to explicitly replace η_{is} by $a^\dagger_{is}$ in equation (4.10) and to re-express the result in terms of η_{is}. From equations (4.4) and (A1.3), it results that such a substitution makes $x_{\alpha\beta}$ vanish identically. In equation (4.10), the summation indices $\lambda_{\alpha\beta}$ must therefore be restricted to zero values:

$$\lambda_{\alpha\beta} = 0 \qquad \alpha = 1, \ldots, p \qquad \beta = 1, \ldots, q. \tag{4.16}$$

By introducing equation (4.16) into equation (4.8), we obtain the following relations:

$$\begin{aligned} j_s &= k_s & s &= 1, \ldots, p \\ &= -k'_{n-s+1} & s &= n-q+1, \ldots, n \end{aligned} \tag{4.17}$$

which, together with equation (4.9), completely determine the U(n) irrep labels in terms of the U(p, q) irrep ones in accordance with the first row of table 1. Equation (4.10) now becomes

$$|\ \rangle = C \prod_{\alpha=1}^{p} (a^\dagger_{p-\alpha+1\ldots p,1\ldots\alpha})^{k_\alpha - k_{\alpha+1}} \sum_{\beta=1}^{q} (a^\dagger_{d-\beta+1\ldots d,n-\beta+1\ldots n})^{k'_\beta - k'_{\beta-1}}|0\rangle \tag{4.18}$$

or

$$|\ \rangle = C \prod_{\alpha=1}^{p} (\eta_{p-\alpha+1\ldots p,1\ldots\alpha})^{k_\alpha - k_{\alpha+1}} \prod_{\beta=1}^{q} (\eta_{d-\beta+1\ldots d,n-\beta+1\ldots n})^{k'_\beta - k'_{\beta+1}}|0\rangle \tag{4.19}$$

where C is some normalisation constant. In deriving equation (4.19) from equation (4.18), we have taken into account that all the terms arising from the second term on the right-hand side of equation (4.14) do vanish.

In conclusion, we have shown that when equations (4.9) and (4.17) hold, the system (3.23) has a unique solution given by equation (4.19).

5. Proof of the complementarity relation when $n < p + q$

In the three cases corresponding to $n < p+q$, we can essentially proceed along the same lines as in the previous section. However, an additional difficulty appears when trying to write the counterpart of equation (4.18) in terms of standard boson operators: the second term on the right-hand side of equation (4.14), which did not have any effect when $n \geqslant p+q$, now cannot be ignored any more. Fortunately, it is possible to avoid calculating its contribution by resorting to a trick, that we shall now proceed to explain.

Let us consider for instance the case where $p \leqslant n < p+q$. The simultaneous solutions of equations (3.23a), (3.23b), (3.23d) and (3.23e) can be written as

$$\begin{aligned} |\ \rangle = &\left(\prod_{\alpha=1}^{n-q} (\eta_{p-\alpha+1\ldots p,1\ldots\alpha})^{j_\alpha - k_{\alpha+1}} \right) \\ &\times \left(\prod_{\beta=1}^{n-p} (\eta_{d-\beta+1\ldots d,n-\beta+1\ldots n})^{-j_{n-\beta+1} - k'_{\beta+1}} \right) \\ &\times \left[\sum_{\{\lambda_{\alpha\beta}\}} C_{\{\lambda_{\alpha\beta}\}} \left(\prod_{\alpha=n-q+1}^{p} (\eta_{p-\alpha+1\ldots p,1\ldots\alpha})^{k_\alpha - k_{\alpha+1} - \Sigma_\beta \lambda_{\alpha\beta}} \right) \right. \\ &\times \left. \left(\prod_{\beta=n-p+1}^{q} (\eta_{d-\beta+1\ldots d,n-\beta+1\ldots n})^{k'_\beta - k'_{\beta+1} - \Sigma_\alpha \lambda_{\alpha\beta}} \right) \prod_{\alpha\beta} (x_{\alpha\beta})^{\lambda_{\alpha\beta}} \right] |0\rangle. \end{aligned} \tag{5.1}$$

In equation (5.1), the indices of the operators $x_{\alpha\beta}$ vary in the range $\alpha = 1, \ldots, p$, $\beta = 1, \ldots, \min(q, n-\alpha)$ and, as a consequence of equation (3.23d), their exponents

$\lambda_{\alpha\beta}$ satisfy the following relations:

$$\begin{aligned}
&\sum_{\beta} \lambda_{s\beta} = k_s - j_s && s = 1, \ldots, n-q \\
&\sum_{\alpha} \lambda_{\alpha,n-s+1} = k'_{n-s+1} + j_s - k_s + \sum_{\beta} \lambda_{s\beta} && s = n-q+1, \ldots, p \\
&\sum_{\alpha} \lambda_{\alpha,n-s+1} = k'_{n-s+1} + j_s && s = p+1, \ldots, n.
\end{aligned} \tag{5.2}$$

As previously, equation (3.23c) is solved by replacing η_{is} by $a^{\dagger}_{is}$ in equation (5.1). This makes $x_{\alpha\beta}$ vanish identically and hence we must restrict the summation indices $\lambda_{\alpha\beta}$ to zero values. From equation (5.2), it results that

$$\begin{aligned}
j_s &= k_s && s = 1, \ldots, n-q \\
&= k_s - k'_{n-s+1} && s = n-q+1, \ldots, p \\
&= -k'_{n-s+1} && s = p+1, \ldots, n.
\end{aligned} \tag{5.3}$$

Equation (5.1) is then transformed into equation (4.18).

From equation (3.23c), it results that

$$2 \sum_{i}{}' \sum_{j}{}'' D^{\dagger}_{ij} D_{ij} | \; \rangle = 0. \tag{5.4}$$

In appendix 2, it is shown that the operator on the left-hand side of this relation can be expressed in terms of the second order Casimir operator of U(n) and of the first and second order Casimir operators of U(p) and U(q). Since the eigenvalues of such operators are well known, equation (5.4) can be rewritten as follows:

$$\begin{aligned}
&\sum_{\alpha=1}^{p} k_\alpha (k_\alpha + n + p - q - 2\alpha + 1) + \sum_{\beta=1}^{q} k'_\beta (k'_\beta + n - p + q - 2\beta + 1) \\
&\qquad - \sum_{s=1}^{n} j_s (j_s + n + p - q - 2s + 1) = 0.
\end{aligned} \tag{5.5}$$

By introducing equation (5.3) into equation (5.5), we obtain for the latter

$$2 \sum_{s=n-q+1}^{p} k_s k'_{n-s+1} = 0. \tag{5.6}$$

Since both k_s and k'_{n-s+1} are non-negative integers, equation (5.6) implies that, for any s in the range $s = n-q+1, \ldots, p$, either k_s or k'_{n-s+1} must vanish. There are $p+q-n+1$ ways of satisfying such conditions, according to the number σ of vanishing k'_{n-s+1}. For any given $\sigma = 0, 1, \ldots, p+q-n$, the following relations hold:

$$\begin{aligned}
k_\alpha &= 0 && \alpha = n-q+\sigma+1, \ldots, p \\
k'_\beta &= 0 && \beta = q-\sigma+1, \ldots, q.
\end{aligned} \tag{5.7}$$

Equation (5.3) now becomes

$$\begin{aligned}
j_s &= k_s && s = 1, \ldots, n-q+\sigma \\
&= -k'_{n-s+1}, && s = n-q+\sigma+1, \ldots, n
\end{aligned} \tag{5.8}$$

showing that σ also determines the relative number of positive and negative labels in $[j_1 \cdots j_n]$. We conclude that the U(n) irrep labels are determined in terms of the U(p, q) irrep labels in accordance with the second row of table 1. Finally, when taking equation (5.7) into account, the substitution of the right-hand side of equation (4.14) for $a^{\dagger}_{is}$ in equation (4.18) is straightforward. It leads to equation (4.19), where the appropriate values of k_α and k'_β have to be set equal to zero in accordance with equation (5.7).

In the two remaining cases $q \leqslant n < p$ and $n < q$, a similar treatment leads to the last two rows of table 1. In each case, the unique solution of equation (3.23) is given by equation (4.19). This completes the proof of the U(p, q)-U(n) complementarity. In the next section, the latter will be illustrated by some examples in atomic physics.

6. Some applications to atomic physics

In recent publications, Kibler and Négadi (1983a, b, 1984) reformulated the known connection between the (three-dimensional) hydrogen atom and a four-dimensional harmonic oscillator with constraint in a way that sheds some light on the hydrogen atom SO(4, 2) dynamical group. The latter was originally described by Barut and Kleinert (1967) as arising from an extension of SO(4, 1). In contrast, Kibler and Négadi obtained it from a constraint on the Sp(8, R) dynamical group of the four-dimensional harmonic oscillator.

Let us show that the analysis of the previous sections provides us with a mathematical formulation of the Kibler-Négadi approach. By setting $p = q = 2$ and $n = 1$ in equation (3.9), we indeed obtain the group chain

$$\mathrm{Sp}(8, R) \supset \mathrm{U}(2,2) = \mathrm{SU}(2,2) \times \mathrm{U}(1) \tag{6.1}$$

where U(2, 2), SU(2, 2) and U(1) are generated by the operators $\mathbb{P}_{i1,j1} = P_{ij}$, $i, j = 1, \ldots, 4$, $P_{ij} - \frac{1}{4} g_{ij} G_1$, $i, j = 1, \ldots, 4$, and G_1 respectively. The above assertion results from the two following properties. First, the Lie algebras of SU(2, 2) and SO(4, 2) are isomorphic. The correspondence between both sets of generators is given in table 2. The SO(4, 2) generators are denoted there by $L_{AB} = -L_{BA} = (L_{AB})^{\dagger}$, $A, B = 1, \ldots, 6$, and they satisfy the following commutation relations:

$$[L_{AB}, L_{CD}] = i(g_{AC}L_{BD} + g_{AD}L_{CB} + g_{BC}L_{DA} + g_{BD}L_{AC}) \tag{6.2}$$

Table 2. Isomorphism between the SO(4, 2) and SU(2, 2) Lie algebras.

SO(4, 2)	SU(2, 2)
$L_+ = L_1 + iL_2 = L_{23} + iL_{31}$	$P_{12} + P_{43}$
$L_- = L_1 - iL_2 = L_{23} - iL_{31}$	$P_{21} + P_{34}$
$L_3 = L_{12}$	$\frac{1}{2}(P_{11} - P_{22} + P_{33} - P_{44})$
$A_+ = A_1 + iA_2 = L_{41} + iL_{42}$	$P_{12} - P_{43}$
$A_- = A_1 - iA_2 = L_{41} - iL_{42}$	$P_{21} - P_{34}$
$A_3 = L_{43}$	$\frac{1}{2}(P_{11} - P_{22} - P_{33} + P_{44})$
$N_+ = N_1 + iN_2 = L_{15} + iL_{25}$	$P_{13} - P_{42}$
$N_- = N_1 - iN_2 = L_{15} - iL_{25}$	$P_{31} - P_{24}$
$N_3 = L_{35}$	$-\frac{1}{2}(P_{14} + P_{23} + P_{32} + P_{41})$
$N_4 = L_{45}$	$\frac{1}{2}i(-P_{14} + P_{23} - P_{32} + P_{41})$
$K_+ = K_1 + iK_2 = L_{16} + iL_{26}$	$i(P_{13} + P_{42})$
$K_- = K_1 - iK_2 = L_{16} - iL_{26}$	$-i(P_{31} + P_{24})$
$K_3 = L_{36}$	$\frac{1}{2}i(-P_{14} - P_{23} + P_{32} + P_{41})$
$K_4 = L_{46}$	$\frac{1}{2}(P_{14} - P_{23} - P_{32} + P_{41})$
$N = L_{56}$	$\frac{1}{2}(P_{11} + P_{22} + P_{33} + P_{44})$

with the metric tensor $g_{AB} = \mathrm{diag}\ (1, 1, 1, 1, -1, -1)$. An alternative notation (Wolf 1967, Moshinsky and Seligman 1981), also used in table 2, is L_a, A_a, N_a, K_a, N_4, K_4, N, $a = 1, 2, 3$, where L_a and A_a are the components of the angular momentum and the Runge-Lenz vector respectively. Second, the U(1) generator, which is the U(2, 2) first order Casimir operator, is

$$G_1 = \eta_{11}\xi_{11} + \eta_{21}\xi_{21} - \eta_{31}\xi_{31} - \eta_{41}\xi_{41}. \tag{6.3}$$

Comparison with the Kibler-Négadi constraint shows that the latter coincides with the relation

$$G_1 = 0. \tag{6.4}$$

In addition, the results of the previous sections enable us to outline some possible extensions of the Kibler-Négadi approach to many-electron atoms. Let us consider n-electron states wherein all the electrons occupy the same shell of the common Coulomb potential. If we set $p = q = 2$ in equation (3.9), we obtain the following group chain:

$$\mathrm{Sp}(8n, R) \supset \mathrm{U}(2n, 2n) \supset \mathrm{SU}(2, 2) \times \mathrm{U}(n) \tag{6.5}$$

where the SU(2, 2) generators are again related to those of SO(4, 2) as shown in table 2. From equation (3.1), it results that SU(2, 2) also belongs to the alternative chain

$$\mathrm{Sp}(8n, R) \supset \mathrm{U}(2n, 2n) \supset \sum_{s=1}^{n} \oplus (\mathrm{SU}(2, 2))_s \supset \mathrm{SU}(2, 2) \tag{6.6}$$

where the intermediate groups $(\mathrm{SU}(2, 2))_s$, $s = 1, \ldots, n$, are generated by the traceless parts of the operators $\mathbb{P}_{is,js}$, $i, j = 1, \ldots, 4$, corresponding to a given s value. Each $(\mathrm{SU}(2, 2))_s$ group is locally isomorphic to an $(\mathrm{SO}(4, 2))_s$ one, whose generators are denoted by $L^{(s)}_{AB}$, or $L^{(s)}_a$, $A^{(s)}_a$, $N^{(s)}_a$, $K^{(s)}_a$, $N^{(s)}_4$, $K^{(s)}_4$, $N^{(s)}$, $a = 1, 2, 3$, and are given in terms of $\mathbb{P}_{is,js}$ by relations similar to those of table 2. Hence the chain (6.6) is equivalent to the chain

$$\sum_{s=1}^{n} \oplus (\mathrm{SO}(4, 2))_s \supset \mathrm{SO}(4, 2). \tag{6.7}$$

In equation (6.7), the SO(4, 2) subgroup generators are given by

$$L_{AB} = \sum_s L^{(s)}_{AB} \tag{6.8a}$$

or

$$\begin{aligned} &L_a = \sum_s L^{(s)}_a \qquad A_a = \sum_s A^{(s)}_a \qquad N_a = \sum_s N^{(s)}_a \qquad K_a = \sum_s K^{(s)}_a \\ &N_4 = \sum_s N^{(s)}_4 \qquad K_4 = \sum_s K^{(s)}_4 \qquad N = \sum_s N^{(s)}. \end{aligned} \tag{6.8b}$$

The SU(2, 2) group appearing in equation (6.5)—or the locally isomorphic SO(4, 2) one—is a dynamical group for the n-electron system. The advantage of chain (6.5) over chain (6.6) or (6.7) is the appearance of the complementary U(n) group, which plays the same role as the Kibler-Négadi constraint for the hydrogen atom.

From equation (6.8), it is obvious that the SO(4, 2) dynamical group for many-electron atoms we are considering here corresponds to an independent-electron picture. Since the underlying SO(4) symmetry is known to be badly broken by the Coulomb interaction between the electrons (Butler and Wybourne 1970, Chacón *et al* 1971), the usefulness for practical purposes of such a dynamical group and, ultimately, that of chain (6.5), may be questioned. For two-electron atoms, however, there is an alternative way of defining the SO(4) symmetry—and the associated SO(4, 2) dynamical group—that incorporates the effects of the Coulomb repulsion between the electrons and enables to predict the mixing coefficients of intrashell doubly excited states with good accuracy (Wulfman and Kumei 1973, Wulfman 1973, Sinanoğlu and Herrick 1975). We shall now show that for such a correlated electron SO(4, 2) dynamical group, a chain similar to equation (6.5), where n is set equal to 2, does also exist.

According to Wulfman and Kumei (1973), the correlated electron SO(4, 2) group, that we shall henceforth denote by $(\mathrm{SO}(4,2))_c$, is the subgroup in the chain

$$(\mathrm{SO}(4,2))_1 \oplus (\mathrm{SO}(4,2))_2 \supset (\mathrm{SO}(4,2)_c \tag{6.9}$$

generated by the operators

$$\begin{array}{lll} L_a^{(c)} = L_a^{(1)} + L_a^{(2)} & A_a^{(c)} = A_a^{(1)} - A_a^{(2)} & N_a^{(c)} = N_a^{(1)} - N_a^{(2)} \\ K_a^{(c)} = K_a^{(1)} - K_a^{(2)} & N_4^{(c)} = N_4^{(1)} + N_4^{(2)} & K_4^{(c)} = K_4^{(1)} + K_4^{(2)} \\ N^{(c)} = N^{(1)} + N^{(2)} & & \end{array} \tag{6.10}$$

To equation (6.9), we can associate the following chain

$$\mathrm{Sp}(16, R) \supset \mathrm{U}(4,4) \supset (\mathrm{SU}(2,2))_1 \oplus (\mathrm{SU}(2,2))_2 \supset (\mathrm{SU}(2,2))_c \tag{6.11}$$

where $(\mathrm{SU}(2,2))_c$ is locally isomorphic to $(\mathrm{SO}(4,2))_c$ and is generated by the traceless parts of the operators $P_{ij}^{(c)}$, $i, j = 1, \ldots, 4$, whose definition in terms of $\mathbb{P}_{is,js}$, $i, j = 1, \ldots, 4$, $s = 1, 2$, is given in table 3. In deriving the latter, we choose the first order Casimir operator of $(\mathrm{U}(2,2))_c$ according to the following prescription:

$$G_1^{(c)} = \mathbb{G}_1^{(1)} - \mathbb{G}_1^{(2)} \tag{6.12}$$

where

$$\mathbb{G}_1^{(s)} = \sum_i \varepsilon_i \mathbb{P}_{is,is} \qquad s = 1, 2 \tag{6.13}$$

are the first order Casimir operators of $(\mathrm{U}(2,2))_s$, $s = 1, 2$.

An analysis of table 3 shows that the operators $P_{ij}^{(c)}$ can be obtained from the operators P_{ij} of equation (3.1) by the substitution of (η_{32}, ξ_{32}), (η_{42}, ξ_{42}), $(-\eta_{12}, -\xi_{12})$,

Table 3. The $(\mathrm{U}(2,2))_c$ generators in terms of the $(\mathrm{U}(2,2))_1 \oplus (\mathrm{U}(2,2))_2$ generators.

$(\mathrm{U}(2,2))_c$	$(\mathrm{U}(2,2))_1 \oplus (\mathrm{U}(2,2))_2$
$P_{11}^{(c)}$	$\mathbb{P}_{11,11} + \mathbb{P}_{32,32}$
$P_{22}^{(c)}$	$\mathbb{P}_{21,21} + \mathbb{P}_{42,42}$
$P_{33}^{(c)}$	$\mathbb{P}_{31,31} + \mathbb{P}_{12,12}$
$P_{44}^{(c)}$	$\mathbb{P}_{41,41} + \mathbb{P}_{22,22}$
$P_{12}^{(c)} = (P_{21}^{(c)})^\dagger$	$\mathbb{P}_{11,21} + \mathbb{P}_{42,32}$
$P_{13}^{(c)} = (P_{31}^{(c)})^\dagger$	$\mathbb{P}_{11,31} - \mathbb{P}_{12,32}$
$P_{14}^{(c)} = (P_{41}^{(c)})^\dagger$	$\mathbb{P}_{11,41} - \mathbb{P}_{22,32}$
$P_{23}^{(c)} = (P_{32}^{(c)})^\dagger$	$\mathbb{P}_{21,31} - \mathbb{P}_{12,42}$
$P_{24}^{(c)} = (P_{42}^{(c)})^\dagger$	$\mathbb{P}_{21,41} - \mathbb{P}_{22,42}$
$P_{34}^{(c)} = (P_{43}^{(c)})^\dagger$	$\mathbb{P}_{31,41} + \mathbb{P}_{22,12}$

$(-\eta_{22}, -\xi_{22})$ for (η_{12}, ξ_{22}), (η_{22}, ξ_{22}), (η_{32}, ξ_{32}), (η_{42}, ξ_{42}), respectively. It is obvious that such a replacement does not change the commutation relations or the Hermiticity properties. Hence, if we perform the same substitution in the U(2) generators $\mathscr{P}_{st}$ of equation (3.2), we obtain new operators $\mathscr{P}_{st}^{(c)}$, given by

$$\begin{aligned}
\mathscr{P}_{11}^{(c)} &= \mathbb{E}_{11,11} + \mathbb{E}_{21,21} - \mathbb{E}_{31,31} - \mathbb{E}_{41,41} \\
\mathscr{P}_{22}^{(c)} &= \mathbb{E}_{32,32} + \mathbb{E}_{42,42} - \mathbb{E}_{12,12} - \mathbb{E}_{22,22} \\
\mathscr{P}_{12}^{(c)} &= (\mathscr{P}_{21}^{(c)})^{\dagger} = \mathbb{E}_{11,32} + \mathbb{E}_{21,42} + \mathbb{E}_{12,31} + \mathbb{E}_{22,41}
\end{aligned} \tag{6.14}$$

and still generating a U(2) group, that we shall denote by $(\mathrm{U}(2))_{\mathrm{c}}$. However, the latter is not a subgroup of U(4, 4), but of the group $(\mathrm{U}(4,4))_{\mathrm{c}}$ resulting from the same substitution. The correlated electron SU(2, 2) group therefore belongs to a chain similar to chain (6.5), where n is set equal to 2, namely

$$\mathrm{Sp}(16, R) \supset (\mathrm{U}(4,4))_{\mathrm{c}} \supset (\mathrm{SU}(2,2))_{\mathrm{c}} \times (\mathrm{U}(2))_{\mathrm{c}}. \tag{6.15}$$

In conclusion, we have shown that the mathematical framework underlying the Kibler–Négadi approach of the hydrogen atom dynamical group can be extended to the independent-electron dynamical group of intrashell many-electron states, as well as to the correlated electron dynamical group of intrashell doubly excited states. In such generalisations, there appears either a $\mathrm{U}(n)$ or a $(\mathrm{U}(2))_{\mathrm{c}}$ group, which is the counterpart of the Kibler–Négadi constraint. At this point, it is worth remembering that a complementarity relation, similar to that between U(2, 2) and $\mathrm{U}(n)$, or $(\mathrm{U}(2,2))_{\mathrm{c}}$ and $(\mathrm{U}(2))_{\mathrm{c}}$, makes its appearance in the theory of nuclear collective states and plays an important role there (Rosensteel and Rowe 1980, Vanagas 1981, Vasilevskii *et al* 1980). In such a theory the complementary groups are the dynamical group $\mathrm{Sp}(6, R)$ of the three-dimensional harmonic oscillator and an $\mathrm{O}(n)$ group, where $n = A - 1$ and A is the nucleon number (Chacón 1969, Moshinsky and Quesne 1971, Deenen and Quesne 1982a, b, 1984). Whether the complementarity relations between U(2, 2) and $\mathrm{U}(n)$, and between $(\mathrm{U}(2,2))_{\mathrm{c}}$ and $(\mathrm{U}(2))_{\mathrm{c}}$, have similar important consequences in atomic physics remains to be investigated.

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Appendix 1. Properties of the traceless boson operators

The purpose of the present appendix is to list various properties of the traceless boson operators $a_{is}^{\dagger}$ and a_{is}, $i = 1, \ldots, d$, $s = 1, \ldots, n$, defined by conditions (4.11) and (4.12), and whose explicit expressions are given in equations (4.13)–(4.15).

In the space of states satisfying equation (4.11), the operators $a_{is}^{\dagger}$ and a_{is} are Hermitian conjugates of one another and satisfy the following commutation relations:

$$[a_{is}, a_{jt}] = [a_{is}^{\dagger}, a_{jt}^{\dagger}] = 0 \tag{A1.1}$$

$$
\begin{aligned}
[a_{is}, a^\dagger_{jt}] &= \delta_{ij}\delta_{st} - \sum_{kl}{}'' a^\dagger_{ks}\Delta^{-1}_{ik,jl} a_{lt} && \text{if } i,j=1,\ldots\ldots,p \\
&= -\sum_k{}''\sum_l{}' a^\dagger_{ks}\Delta^{-1}_{ik,lj} a_{lt} && \text{if } i=1,\ldots,p \qquad j=p+1,\ldots,d \\
&= -\sum_k{}'\sum_l{}'' a^\dagger_{ks}\Delta^{-1}_{ki,jl} a_{lt} && \text{if } i=p+1,\ldots,d \qquad j=1,\ldots,p \\
&= \delta_{ij}\delta_{st} - \sum_{kl}{}' a^\dagger_{ks}\Delta^{-1}_{ki,lj} a_{lt} && \text{if } i,j=p+1,\ldots,d.
\end{aligned} \tag{A1.2}
$$

Moreover, they fulfil the traceless conditions

$$
\sum_s a^\dagger_{is} a^\dagger_{js} = 0 \qquad i=1,\ldots,p \qquad j=p+1,\ldots,d. \tag{A1.3}
$$

The proofs of equations (A1.1)-(A1.3) are quite similar to those given by Lohe and Hurst (1971) for O(n) or USp(n) traceless boson operators and will therefore be omitted. Equations (A1.2) show that the operators $a^\dagger_{is}$, a_{is} are not true boson operators, but modified ones, while equation (A1.3) accounts for their name of traceless boson operators.

Next let us prove that when η_{is} is replaced by $a^\dagger_{is}$ in any simultaneous solution of equations (3.23a), (3.23b), (3.23d) and (3.23e), the resulting state remains a solution of these equations and, in addition, satisfies equation (3.23c). The latter point directly results from the defining property (4.12) of the traceless boson operators and the fact that the vacuum state $|0\rangle$ satisfies equation (4.11). The proof of the former point goes in two steps. First, we note that in the space of states satisfying equation (4.11), the U(p) × U(q) and U(n) generators have similar expressions in terms of the traceless and the standard boson operators:

$$
\sum_s a^\dagger_{is} a_{js} = \sum_s \eta_{is}\xi_{js} \qquad i,j=1,\ldots,p \text{ or } i,j=p+1,\ldots,d \tag{A1.4}
$$

$$
\sum_i{}' a^\dagger_{is} a_{it} - \sum_i{}'' a^\dagger_{it} a_{is} = \sum_i{}' \eta_{is}\xi_{it} - \sum_i{}'' \eta_{it}\xi_{is} \qquad s,t=1,\ldots,n. \tag{A1.5}
$$

Equations (A1.4) and (A1.5) are easily demonstrated by using equations (4.11), (4.13) and (4.14). Second, in the same space, both the traceless and the standard boson operators behave in the same way under U(p) × U(q) and U(n). By applying equations (A1.1)-(A1.3), the following relations:

$$
\left(\sum_s a^\dagger_{is} a_{js}, a^\dagger_{kt}\right) = \delta_{jk} a^\dagger_{it} \qquad i,j=1,\ldots,p \text{ or } i,j=p+1,\ldots,d \qquad k=1,\ldots,d \qquad t=1,\ldots,n \tag{A1.6}
$$

and

$$
\begin{aligned}
&\left(\sum_i{}' a^\dagger_{is} a_{it} - \sum_i{}'' a^\dagger_{it} a_{is}, a^\dagger_{ju}\right) \\
&\qquad = \delta_{tu} a^\dagger_{js} \qquad \text{if } j=1,\ldots,p \qquad s,t,u=1,\ldots,n \\
&\qquad = -\delta_{su} a^\dagger_{jt} \qquad \text{if } j=p+1,\ldots,d \qquad s,t,u=1,\ldots,n
\end{aligned} \tag{A1.7}
$$

are indeed easily proved. This completes the demonstration of the above assertion.

Appendix 2. Second order Casimir operators of $\mathrm{U}(p, q)$ and $\mathrm{U}(n)$

In the present appendix, we shall show that the second order Casimir operators of $\mathrm{U}(p, q)$ and $\mathrm{U}(n)$ are linearly related and consequently that equations (5.4) and (5.5) are equivalent.

The second order Casimir operators of $\mathrm{U}(p, q)$ and $\mathrm{U}(n)$ are defined by

$$G_2 = \sum_{ij} \varepsilon_i \varepsilon_j P_{ij} P_{ji} \tag{A2.1}$$

and

$$\mathscr{G}_2 = \sum_{st} \mathscr{P}_{st} \mathscr{P}_{ts} \tag{A2.2}$$

respectively. By using equations (3.3) and (3.12), G_2 can be rewritten as

$$G_2 = -2 \sum_i{}' \sum_j{}'' D^\dagger_{ij} D_{ij} + \Phi_2^{(p)} + \Phi_2^{(q)} - q\Phi_1^{(p)} - p\Phi_1^{(q)} \tag{A2.3}$$

where

$$\Phi_1^{(p)} = \sum_i{}' E_{ii} \qquad \Phi_1^{(q)} = \sum_i{}'' E_{ii} \tag{A2.4}$$

and

$$\Phi_2^{(p)} = \sum_{ij}{}' E_{ij} E_{ji} \qquad \Phi_2^{(q)} = \sum_{ij}{}'' E_{ij} E_{ji} \tag{A2.5}$$

are, respectively, the first order and the second order Casimir operators of $\mathrm{U}(p)$ and $\mathrm{U}(q)$. In the same way, by applying equations (2.2), (2.4) and (3.2), $\mathscr{G}_2$ can be put into the following form:

$$\mathscr{G}_2 = \sum_{st} \left(\sum_{ij}{}' \mathbb{E}_{is,it} \mathbb{E}_{jt,js} - 2 \sum_i{}' \sum_j{}'' \mathbb{E}_{is,it} \mathbb{E}_{js,jt} + \sum_{ij}{}'' \mathbb{E}_{is,it} \mathbb{E}_{jt,js} \right). \tag{A2.6}$$

Let us now introduce equations (2.1) and (3.11) into equations (A2.3) and (A2.6). By reordering the boson creation and annihilation operators, one easily obtains the following linear relation between G_2 and $\mathscr{G}_2$:

$$G_2 - \mathscr{G}_2 = \tfrac{1}{4} n(p+q)(n-p-q). \tag{A2.7}$$

From equations (A2.3) and (A2.7), the operator $2 \Sigma_i' \Sigma_j'' D^\dagger_{ij} D_{ij}$ can be expressed as

$$2 \sum_i{}' \sum_j{}'' D^\dagger_{ij} D_{ij} = \Phi_2^{(p)} + \Phi_2^{(q)} - q\Phi_1^{(p)} - p\Phi_1^{(q)} - \mathscr{G}_2 - \tfrac{1}{4} n(p+q)(n-p-q). \tag{A2.8}$$

Since the solutions $|\ \rangle$ of equations (3.23) transform according to the irreps (3.18) of $\mathrm{U}(n)$, $\{k_1 + n/2, \ldots, k_p + n/2\}$ of $\mathrm{U}(p)$, and $\{k'_1 + n/2, \ldots, k'_q + n/2\}$ of $\mathrm{U}(q)$, the corresponding eigenvalues of the $\mathrm{U}(n)$, $\mathrm{U}(p)$ and $\mathrm{U}(q)$ Casimir operators are easily obtained. For $\mathrm{U}(p)$, for instance, they are given by (Louck 1970)

$$\begin{aligned} \Phi_1^{(p)} |\ \rangle &= \sum_{\alpha=1}^{p} (k_\alpha + n/2) |\ \rangle \\ \Phi_2^{(p)} |\ \rangle &= \sum_{\alpha=1}^{p} (k_\alpha + n/2)(k_\alpha + n/2 + p - 2\alpha + 1) |\ \rangle. \end{aligned} \tag{A2.9}$$

By using equations (A2.8), (A2.9) and similar relations for $\mathrm{U}(n)$ and $\mathrm{U}(q)$, it is straightforward to transform equation (5.4) into equation (5.5).

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