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Products and plethysms for the fundamental harmonic series representations of $U(p, q)$

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Abstract. We give the decomposition of the Kronecker products and the symmetrized Kronecker squares of all the fundamental representations of the harmonic series of unitary irreducible representations of $U(p, q)$. The results for $U(2, 2)$ are relevant to two-electron hydrogenic-like atoms.

1. Introduction

Bohr, in his very first paper [3], on what has become known as ‘The Bohr-model’ of the atom, made the surprising discovery that the energies of levels of the non-relativistic hydrogen atom could be expressed (in appropriate units) as simply

$$E_n = -\frac{1}{n^2} \quad \text{with } n = 0, 1, 2, \dots$$

With the advent of the Schrödinger equation for the H atom it became apparent that each value of n could be associated with orbital angular momenta of

$$\ell = 0, 1, 2, \dots, n - 1$$

and associated with each value of ℓ there were $(2\ell + 1)$ values of the angular momentum projection eigenvalues m_ℓ leading to each energy level E_n being associated with $(n - 1)^2$ eigenfunctions. Initially, such a high degeneracy appeared surprising. Pauli [7] noted that in a purely Coulombic central field there was an additional constant of motion associated with the Runge–Lenz vector and from there it led to the realization that the observed degeneracies were precisely the dimensions of certain irreducible representations of the group $SO(4) \sim SU(2) \times SU(2)$, in particular those commonly designated as $[n - 1, 0] \sim \{n - 1\} \times \{n - 1\}$.

Many years later, Barut and Kleinert [2] observed that all the discrete levels of a H atom spanned a single infinite-dimensional irreducible representation of the non-compact group $SO(4, 2) \sim SU(2, 2)$ with the group being referred to as the *dynamical group* of the H atom [2, 9]. The Runge–Lenz vector ceases to be a constant of motion for two or more electrons in a central Coulomb field [2, 9, 10, 4] and the $SO(4)$ symmetry is broken. Nevertheless, it can be useful to consider the n -electron states starting with the single irreducible representation of $SU(2, 2)$, or more simply $U(2, 2)$, and then forming symmetrized n -fold tensor products which will be the central problem considered here. For greater generality we shall initially consider the group $U(p, q)$ as previously studied by King and Wybourne [6]. After a

brief sketch of the relevant properties of $U(p, q)$ we tackle the problem of resolving the Kronecker powers of the relevant irreducible representation into its relevant symmetrized powers, namely the problem of plethysms in $U(p, q)$. In the process we are able to give closed results for the second powers of the fundamental harmonic series irreducible representations of $U(p, q)$ which thus yields, in the case of two electrons, the appropriate spin triplet and singlet states.

2. The fundamental harmonic series irreducible representations of $U(p, q)$

Following [6], we may embed the non-compact group $U(p, q)$ into $Sp(2p + 2q, R)$ whose harmonic representation $\tilde{\Delta}$ decomposes as

$$\tilde{\Delta} \rightarrow H = H_0 + \sum_{m=1}^{\infty} (H_m + H_{-m}) \quad (1)$$

where

$$H_0 = \{1(\bar{0}; 0)\} \quad (2a)$$

$$H_m = \{1(\bar{0}; m)\} \quad m = 1, 2, \dots \quad (2b)$$

$$H_{-m} = \{1(\bar{m}; 0)\} \quad m = 1, 2, \dots \quad (2c)$$

Upon restriction to the maximal compact subgroup $U(q) \times U(p)$ we have

$$H_0 = \{1(\bar{0}; 0)\} \rightarrow (0 \times \varepsilon) \left(\sum_{j=0}^{\infty} \{\bar{j}\} \times \{j\} \right) \quad (3a)$$

$$H_m = \{1(\bar{0}; m)\} \rightarrow (0 \times \varepsilon) \left(\sum_{j=0}^{\infty} \{\bar{j}\} \times \{m + j\} \right) \quad (3b)$$

$$H_{-m} = \{1(\bar{m}; 0)\} \rightarrow (0 \times \varepsilon) \left(\sum_{j=0}^{\infty} \{\overline{m+j}\} \times \{j\} \right). \quad (3c)$$

The harmonic series unitary irreducible representations (abbreviated to unirreps) $\{k(\bar{\nu}; \mu)\}$ of $U(p, q)$ are generated by considering powers [5] H^k of H . Under restriction from $U(pk, qk)$ to $U(p, q) \times U(k)$

$$H \rightarrow \sum_{\nu, \mu} \{k(\bar{\nu}; \mu)\} \times \{\bar{\nu}; \mu\} \quad (4)$$

where the conjugate partitions $(\bar{\nu})$ and $(\bar{\mu})$ satisfy the constraints [5]

$$\tilde{\mu}_1 + \tilde{\nu}_1 \leq k \quad (5a)$$

$$\tilde{\mu}_1 \leq p \quad \text{and} \quad \tilde{\nu}_1 \leq q. \quad (5b)$$

3. Kronecker products for all of the fundamental harmonic series unirreps

The Kronecker product of two arbitrary unirreps of $U(p, q)$ may be evaluated following [6] to give

$$\{k(\bar{\nu}; \mu)\} \times \{\ell(\bar{\tau}; \sigma)\} = \sum_{\zeta} \{k + \ell(\{\bar{\nu}_s\}^k \{\bar{\tau}_s\}^{\ell} \{\bar{\zeta}\}; \{\mu_s\}^k \{\sigma_s\}^{\ell} \{\zeta\})\} \quad (6)$$

where the notation is as in [6] and it is understood that

$$(\bar{\rho}; \lambda)_{k+\ell, p, q} = \begin{cases} (\bar{\rho}; \lambda) & \text{if } \tilde{\lambda}_1 \leq p, \tilde{\rho}_1 \leq q \text{ and } \tilde{\lambda}_1 + \tilde{\rho}_1 \leq k + \ell \\ 0 & \text{otherwise.} \end{cases} \quad (7)$$

Specialization of (6) to the fundamental harmonic series of $U(p, q)$ yields the following cases: for $m, r, s > 0$,

$$H_0^2 = \sum_{n=0}^{\infty} \{2(\bar{n}; n)\} \tag{8a}$$

$$H_m^2 = \sum_{n=0}^{\infty} \{2(\bar{n}; n + 2m)\} + \sum_{p=1}^m \{2(\bar{0}; 2m - p, p)\} \tag{8b}$$

$$H_{-m}^2 = \sum_{n=0}^{\infty} \{2(\overline{n + 2m}; n)\} + \sum_{p=1}^m \{2(\overline{2m - p}; p; 0)\} \tag{8c}$$

$$H_m \times H_{-m} = \sum_{k=0}^{\infty} \{2(\overline{m + k}; m + k)\} \tag{8d}$$

$$H_r \times H_s = \sum_{x=0}^{\min(r,s)} \{2(\bar{0}; r + s - x, x)\} + \sum_{k=1}^{\infty} \{2(\bar{k}; r + s + k)\} \tag{8e}$$

$$H_{-r} \times H_{-s} = \sum_{x=0}^{\min(r,s)} \{2(\overline{r + s - x}; x; 0)\} + \sum_{k=1}^{\infty} \{2(\overline{r + s + k}; k)\} \tag{8f}$$

$$H_{-r} \times H_s = \{2(\bar{r}; s)\} + \sum_{k=1}^{\infty} \{2(\overline{r + k}; s + k)\} \tag{8g}$$

$$H_0 \times H_m = \{2(\bar{0}; m)\} + \sum_{k=1}^{\infty} \{2(\bar{k}; m + k)\} \tag{8h}$$

$$H_0 \times H_{-m} = \{2(\bar{m}; 0)\} + \sum_{k=1}^{\infty} \{2(\overline{m + k}; k)\}. \tag{8i}$$

4. Symmetrized squares of the fundamental harmonic representations

To separate the Kronecker squares of the representations H_m of $U(p, q)$ into its symmetric and antisymmetric parts, we first solve the corresponding problem for the complete harmonic representation H . This is done by restricting the H of $U(2p, 2q)$ through the chain

$$U(2p, 2q) \supset U(p, q) \times U(2) \supset U(p, q) \times S_2 \supset U(p, q). \tag{9}$$

Under $U(2p, 2q) \downarrow U(p, q) \times U(2)$, equation (4), and constraints (5a) and (5b) with $k = 2$ yield

$$H \rightarrow \sum_{\bar{v}_1 + \bar{\mu}_1 \leq 2} \{2(\bar{v}; \mu)\} \times \{\bar{v}; \mu\}. \tag{10}$$

Therefore, we just have to determine the restriction to S_2 of the $U(2)$ representations $\{\bar{v}; \mu\}$.

It is known ([1], see also [8]) that the Frobenius characteristic of the decomposition of $\{m\}$ under $U(k) \downarrow S_k$ is the coefficient of z^m in the series

$$h_k \left(\frac{X}{1-z} \right) = \prod_{j=1}^k \frac{1}{1-z^j} \sum_{\lambda \vdash k} \tilde{K}_{\lambda, 1^k}(z) s_{\lambda} \tag{11}$$

where $\tilde{K}_{\lambda, 1^k}(z)$ are the (cocharge) Kostka–Foulkes polynomials. In particular, for $k = 2$, $\{m\} \downarrow S_2$ is the coefficient of z^m in

$$\frac{1}{(1-z)(1-z^2)} [(2) + z(11)] \tag{12}$$

so that

$$\{m\} \rightarrow p_2(m)(2) + p_2(m - 1)(11) \tag{13}$$

where $p_2(m)$ is the number of partitions of m into parts not greater than 2, that is, $p_2(m) = \lceil \frac{m+1}{2} \rceil$.

Taking into account the $U(2)$ equivalences $\{\bar{0}; \mu_1 \mu_2\} \equiv \epsilon^{\mu_2} \{\mu_1 - \mu_2\}$, $\{\bar{m}; n\} \equiv \epsilon^{-m} \{n + m\}$ and $\{\bar{v}_1 \bar{v}_2; 0\} \equiv \epsilon^{-v_1} \{v_1 - v_2\}$, we obtain

$$\{\bar{0}; \mu_1 \mu_2\} \rightarrow \begin{cases} p_2(\mu_1 - \mu_2)(2) + p_2(\mu_1 - \mu_2 - 1)(11) & \text{for } \mu_2 \text{ even} \\ p_2(\mu_1 - \mu_2 - 1)(2) + p_2(\mu_1 - \mu_2)(11) & \text{for } \mu_2 \text{ odd} \end{cases} \tag{14a}$$

$$\{\bar{m}; n\} \rightarrow \begin{cases} p_2(m + n)(2) + p_2(m + n - 1)(11) & \text{for } m \text{ even} \\ p_2(m + n - 1)(2) + p_2(m + n)(11) & \text{for } m \text{ odd} \end{cases} \tag{14b}$$

$$\{\bar{v}_1 \bar{v}_2; 0\} \rightarrow \begin{cases} p_2(v_1 - v_2)(2) + p_2(v_1 - v_2 - 1)(11) & \text{for } v_1 \text{ even} \\ p_2(v_1 - v_2 - 1)(2) + p_2(v_1 - v_2)(11) & \text{for } v_1 \text{ odd.} \end{cases} \tag{14c}$$

Now, we have

$$\begin{aligned} H \otimes \{2\} &= \left(H_0 + \sum_{m=1}^{\infty} (H_m + H_{-m}) \right) \otimes \{2\} = H_0 \otimes \{2\} + H_0 \times \sum_{m=1}^{\infty} (H_m + H_{-m}) \\ &+ \left(\sum_{m=1}^{\infty} H_m \right) \otimes \{2\} + \sum_{r,s=1}^{\infty} H_r \times H_{-s} + \left(\sum_{m=1}^{\infty} H_{-m} \right) \otimes \{2\} = H_0 \otimes \{2\} \\ &+ \sum_{m=1}^{\infty} H_m \times H_{-m} + R. \end{aligned}$$

To extract $H_0 \otimes \{2\}$ from $H \otimes \{2\}$, we remark that since under $U(p, q) \downarrow U(p) \times U(q)$

$$H_0 \rightarrow (0 \times \epsilon) \sum_{m=0}^{\infty} \{\bar{m}\} \times \{m\}$$

the Kronecker square of H_0 can only contain terms whose restriction to $U(p) \times U(q)$ is a sum of representations $(0 \times \epsilon^2) \{\bar{v}; \mu\}$ such that $|v| = |\mu|$. Clearly, the terms in R are not of this form, and to obtain $H_0 \otimes \{2\}$, we just need to compute the terms of the form $\{2(\bar{m}; m)\}$ in $H \otimes \{2\}$ and to remove the contribution of $\sum_{m=1}^{\infty} H_m \times H_{-m}$.

We know from the above discussion that the multiplicity of $\{2(\bar{m}; m)\}$ in $H \otimes \{2\}$ is equal to $p_2(m + m) = m + 1$ for m even, and to $p_2(m + m - 1) = m$ for m odd. On the other hand,

$$H_m \times H_{-m} = \sum_{k=0}^{\infty} \{2(\overline{m+k}; m+k)\}$$

so that a given $\{2(\bar{m}; m)\}$ occurs exactly m times in $\sum_{k=1}^{\infty} H_k \times H_{-k}$. Removing this contribution, we are left with

$$H_0 \otimes \{2\} = \sum_{k=0}^{\infty} \{2(2\bar{k}; 2k)\}. \tag{15}$$

Since $H_0^2 = \sum_{m=0}^{\infty} \{2(\bar{m}; m)\}$, we also have

$$H_0 \otimes \{1^2\} = \sum_{k=0}^{\infty} \{2(\overline{2k+1}; 2k+1)\}. \tag{16}$$

To split the square of H_m ($m \geq 1$), we first observe that under restriction to $U(p) \times U(q)$, it yields a sum of representations of the form $(0 \times \epsilon^2)\{\bar{\nu}\} \times \{\mu\}$ such that $|\mu| = |\nu| + 2m$. Next, we proceed as above to extract it from $H \otimes \{2\}$. We have

$$H \otimes \{2\} = \left(H_m + \sum_{j \neq m} H_j \right) \otimes \{2\} = H_m \otimes \{2\} + H_m \times \sum_{j \neq m} H_j + \left(\sum_{j=1}^{\infty} H_{m-j} \right) \otimes \{2\} \\ + \left(\sum_{j=1}^{\infty} H_{m-j} \right) \times \left(\sum_{k=1}^{\infty} H_{m+k} \right) + \left(\sum_{j=1}^{\infty} H_{m+j} \right) \otimes \{2\}.$$

Therefore, to extract $H_m \otimes \{2\}$, we just have to select from $H \otimes \{2\}$ the terms having the correct restriction property to $U(p) \times U(q)$ and to subtract the contribution of the crossed products $H_{m-j} \times H_{m+j}$ ($j \geq 1$). Suppose first that $m \geq 1$, then,

$$\sum_{j=1}^{\infty} H_{m-j} \times H_{m+j} = H_0 \times H_{2m} + \sum_{r=1}^{m-1} H_r \times H_{2m-r} + \sum_{r=1}^{\infty} H_{-r} \times H_{2m+r}. \tag{17}$$

The terms of this sum are

$$H_0 \times H_{2m} = \sum_{k=0}^{\infty} \{2(\bar{k}; 2m + k)\} \tag{18a}$$

$$H_r \times H_{2m-r} = \sum_{i=1}^r \{2(\bar{0}; 2m - i, i)\} + \sum_{k=0}^{\infty} \{2(\bar{k}; 2m + k)\} \tag{18b}$$

$$H_{-r} \times H_{2m+r} = \sum_{k=0}^{\infty} \{2(\overline{r+k}, 2m + r + k)\} \tag{18c}$$

so that

$$\sum_{j=1}^{\infty} H_{m-j} \times H_{m+j} = \sum_{i=1}^{m-1} (m - i) \{2(\bar{0}; 2m - i, i)\} + \sum_{k=0}^{\infty} (m + k) \{2(\bar{k}; 2m + k)\}. \tag{19}$$

Now, the multiplicity of $\{2(\bar{0}; 2m - i, i)\}$ in $H \otimes \{2\}$ is $p_2(2m - 2i) = m - i + 1$ for i even, and $p_2(2m - 2i - 1) = m - i$ for i odd. Similarly, the multiplicity of $\{2(\bar{k}; 2m + k)\}$ in $H \otimes \{2\}$ is equal to $p_2(2m + 2k) = m + k + 1$ for k even, and to $p_2(2m + 2k - 1) = m + k$ for k odd. Finally, we are left with

$$H_m \otimes \{2\} = \sum_{i=1}^{\lfloor m/2 \rfloor} \{2(\bar{0}; 2m - 2i, 2i)\} + \sum_{k=0}^{\infty} \{2(\overline{2k}; 2m + 2k)\}. \tag{20a}$$

Similarly, we obtain

$$H_m \otimes \{1^2\} = \sum_{i=0}^{\lfloor (m-1)/2 \rfloor} \{2(\bar{0}; 2m - 2i - 1, 2i + 1)\} + \sum_{k=0}^{\infty} \{2(\overline{2k+1}; 2m + 2k + 1)\}. \tag{20b}$$

Likewise,

$$H_{-m} \otimes \{2\} = \sum_{i=1}^{\lfloor m/2 \rfloor} \{2(\overline{2m - 2i}, 2i; 0)\} + \sum_{k=0}^{\infty} \{2(\overline{2m + 2k}; 2k)\} \tag{20c}$$

$$H_{-m} \otimes \{1^2\} = \sum_{i=0}^{\lfloor (m-1)/2 \rfloor} \{2(\overline{2m - 2i - 1}, 2i + 1; 0)\} + \sum_{k=0}^{\infty} \{2(\overline{2m + 2k + 1}; 2k + 1)\}. \tag{20d}$$

5. Conclusion

We have been able to obtain complete results for all the Kronecker products, and their symmetrized squares, for all the fundamental harmonic unirreps of $U(p, q)$ expressing them in a compact closed form. The plethysms of the square of the unirrep H_0 for $U(2, 2)$ give the complete set of $U(2, 2)$ unirreps that arise in a two-electron hydrogenic-like atom with the symmetric part describing the spin singlets ($S = 0$) and the antisymmetric part the spin triplets ($S = 1$). The groundstate $1s^2(^1S)$ is the first level of an infinite tower of states associated with the $\{2(0; 0)\}$ unirrep while the lowest 3SP level is the first level of an infinite tower associated with the $\{2(\bar{1}; 1)\}$ unirrep. A complete account of the two-electron hydrogen-like states remains to be considered but knowing the relevant $U(2, 2)$ unirreps is a significant beginning. For an n -electron hydrogen-like atom ($n > 2$) the resolution of plethysms of the type $H_0 \otimes \{\lambda\}(\lambda \vdash n)$ is a formidable task and complete results of the type considered herein cannot be expected.

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