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

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

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

$$\ell = 1, 2, \ldots, n-1$$

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 the motion associated with the Runge-Lenz vector and from there was led to the realisation that the observed degeneracies were precisely the dimensions of certain of the irreducible

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representations of the group $SO(4) \sim SU(2) \times SU(2)$, in particular those commonly designated as $[n-1,0] \sim \{n-1\} \times \{n-1\}$.

Much 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 the 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 [6] by King and Wybourne. 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 $U(p,q)$ in $Sp(2p+2q,R)$ whose harmonic representation $\tilde{\Delta}$ decomposes as

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

where

$$\begin{aligned} H_0 &= \{1(\bar{0};0)\} && (2a)\\ H_m &= \{1(\bar{0};m)\} \quad m=1,2,\ldots && (2b)\\ H_{-m} &= \{1(\bar{m};0)\} \quad m=1,2,\ldots && (2c)\end{aligned}$$

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

$$H_0 = \{1(\bar{0};0\} \qquad \to (0 \times \varepsilon) \cdot (\sum_{k=0}^{\infty}\{\bar{k}\} \times \{k\}) \tag{3a}$$

$$H_m = \{1(\bar{0};m)\} \quad \to (0 \times \varepsilon) \cdot (\sum_{k=0}^{\infty}\{\bar{k}\} \times \{m+k\}) \tag{3b}$$

$$H_{-m} = \{1(\bar{m};0)\} \to (0 \times \varepsilon) \cdot (\sum_{k=0}^{\infty}\{\overline{m+k}\} \times \{k\}) \tag{3c}$$

The harmonic series 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 $U(p,q)\times U(k)$

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

where the partition (μ) has not more than p parts and (ν) not more than q parts and their conjugate partitions $(\tilde{\nu})$ and $(\tilde{\mu})$ satisfy the constraints [5]

$$\tilde{\mu}_1+\tilde{\nu}_1 \le k \tag{5a}$$

$$\tilde{\mu}_1 \quad \le p \quad \text{and} \quad \tilde{\nu}_1 \le q \tag{5b}$$

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

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

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

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

Specialization of (6) to the fundamental harmonic series of $U(p,q)$ yields the following cases

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

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

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

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

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

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

$$H_{-r}\times H_s = \{2(\bar{r};s)\}+\sum_{k=1}^{\infty}\{2(\overline{r+k};s+k)\} \quad r,s>0 \tag{8g}$$

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

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

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

$$U(2p,2q) \supset U(p,q) \times U(2) \supset U(p,q) \times S_2 \supset U(p,q) \; . \qquad (9)$$

Under $U(2p,2q) \downarrow U(p,q) \times U(2)$, we know that

$$H \to \sum_{\tilde{\nu_1}+\tilde{\mu_1} \leq 2} \{2(\bar{\nu};\mu)\} \times \{\bar{\nu};\mu\} \; . \qquad (10)$$

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

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

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

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

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

so that

$$\{m\} \to p_2(m)(2) + p_2(m-1)(11) \qquad (13)$$

where $p_2(m)$ is the number of partitions of m into parts not greater that 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 $\{\overline{\nu_1\nu_2};0\} \equiv \epsilon^{-\nu_1}\{\nu_1-\nu_2\}$, we obtain

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

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

$$\{\overline{\nu_1\nu_2};0\} \to \begin{cases} p_2(\nu_1-\nu_2)(2) + p_2(\nu_1-\nu_2-1)(11) & \text{for} \quad \nu_1 \text{ even} \\ p_2(\nu_1-\nu_2-1)(2) + p_2(\nu_1-\nu_2)(11) & \text{for} \quad \nu_1 \text{ odd} \end{cases} \qquad (14c)$$

Now, we have

$$H \otimes \{2\} = \left(H_0 + \sum_{m\geq 1} (H_m + H_{-m}) \right) \otimes \{2\}$$

$$= H_0 \otimes \{2\} + H_0 \times \sum_{m\geq 1} (H_m + H_{-m}) + \left(\sum_{m\geq 1} H_m \right) \otimes \{2\}$$

$$+ \sum_{r,s\geq 1} H_r \times H_{-s} + \left(\sum_{m\geq 1} H_{-m} \right) \otimes \{2\}$$

$$= H_0 \otimes \{2\} + \sum_{m\geq 1} H_m \times H_{-m} + R \ .$$

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

$$H_0 \to (0 \times \epsilon) \sum_{m\geq 0} \{\bar{m}\} \times \{m\}$$

the Kronecker square of H_0 can only contain terms whose restriction to $U(p) \times U(q)$ is a sum of representations $(0 \times \epsilon^2)\{\bar{\nu};\mu\}$ such that $|\nu| = |\mu|$. 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 $\sum_{m\geq 1} H_m \times H_{-m}$.

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,

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

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

$$H_0 \otimes \{2\} = \sum_{k\geq 0} \{2(\overline{2k}; 2k)\} \ . \tag{15}$$

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

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

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

$$H \otimes \{2\} = \left(H_m + \sum_{j\neq m} H_j \right) \otimes \{2\}$$

$$= H_m \otimes \{2\} + H_m \times \sum_{j\neq m} H_j + \left(\sum_{j\geq 1} H_{m-j} \right) \otimes \{2\}$$

$$+\left(\sum_{j\geq 1} H_{m-j}\right)\times\left(\sum_{k\geq 1} H_{m+k}\right)+\left(\sum_{j\geq 1} H_{m+j}\right)\otimes\{2\}$$

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,

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

The terms of this sum are

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

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

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

so that

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

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

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

Similarly, we obtain

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

Likewise,

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

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

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 $\{2(\bar{0};0)\}$ 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 $U(2,2)$ unirepps is a significant beginning. For an $n-$electron hydrogen-like atom ($n>2$) the resolution of plethysms of the type $H_0 \otimes \{\lambda\} \quad (\lambda \vdash n)$ is a formidable task and complete results of the type considered herein cannot be expected.

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