PHYSICS 220 : GROUP THEORY
FINAL EXAMINATION

This exam is due in my office, 5438 Mayer Hall, at 10 am, Friday, June 15. You are allowed to use the course lecture notes, the Lax text, and the character tables (link from lecture notes web page), but no other sources, and please do not discuss the exam with anyone other than me. If you have any urgent questions regarding the exam, send me email.

[1] Show that the Lie algebra structure constants are given by the expression

$$f_{ab}{}^c = \left(\frac{\partial S_b{}^c}{\partial x^a}\bigg|_{\boldsymbol{x}_e} - \frac{\partial S_a{}^c}{\partial x^b}\bigg|_{\boldsymbol{x}_e} \right) \quad ,$$

where

$$S_a{}^b(\boldsymbol{x}) = \frac{\partial f^b(\boldsymbol{x},\boldsymbol{u})}{\partial x^a}\bigg|_{\boldsymbol{u}=\boldsymbol{x}^{-1}} \quad ,$$

with $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{y})$ the group composition function. Thus, the structure constants depend on the parameterization of the associated Lie group G, but are representation-independent.

Solution :

Let $D(\boldsymbol{x}) = D(g(\boldsymbol{x}))$ be a representation of G. From the relation $\frac{\partial D}{\partial x^b} = S_b{}^c \, X_c \, D$ we derive

$$\frac{\partial}{\partial x^a}\left[\frac{\partial D}{\partial x^b}\, D^{-1}\right] - \frac{\partial}{\partial x^b}\left[\frac{\partial D}{\partial x^a}\, D^{-1}\right] = \frac{\partial D}{\partial x^b}\,\frac{\partial D^{-1}}{\partial x^a} - \frac{\partial D}{\partial x^a}\,\frac{\partial D^{-1}}{\partial x^b}$$
$$= \left(\frac{\partial S_b{}^c}{\partial x^a} - \frac{\partial S_a{}^c}{\partial x^b}\right) X_c$$

On the other hand, since $D(\boldsymbol{x})D^{-1}(\boldsymbol{x}) = \mathbb{1}$ for all $\boldsymbol{x}$, taking the differential we have $dD^{-1} = -D^{-1}\,(dD)\,D^{-1}$, and the above equation becomes

$$\frac{\partial D}{\partial x^a}\, D^{-1}\, \frac{\partial D}{\partial x^b}\, D^{-1} - \frac{\partial D}{\partial x^b}\, D^{-1}\, \frac{\partial D}{\partial x^a}\, D^{-1} = \left(\frac{\partial S_b{}^c}{\partial x^a} - \frac{\partial S_a{}^c}{\partial x^b}\right) X_c \quad .$$

Now evaluate the above equation at $\boldsymbol{x} = \boldsymbol{x}_e$ to obtain the result

$$\big[X_a \, , \, X_b\big] = f_{ab}{}^c \, X_c$$

where

$$f_{ab}{}^c = \left(\frac{\partial S_b{}^c}{\partial x^a}\bigg|_{\boldsymbol{x}_e} - \frac{\partial S_a{}^c}{\partial x^b}\bigg|_{\boldsymbol{x}_e} \right) \quad .$$

We see that the structure constants are independent of the representation D, but are dependent on the coordinatization of G.

[2] Consider a chromium ion in a D_{3d} environment.

(a) First consider the case of Cr^{2+}, with electronic configuration $[\mathrm{Ar}]\,3\mathrm{d}^4$. Hund's first two rules say that $S = 2$ and $L = 2$ (D). According to Hund's third rule, what is the atomic ground state term?

(b) The character table for the double group D'_{3d} is given in Tab. 1. With an even number of electrons, only the unbarred elements, which comprise D_{3d}, need be considered[1]. Ignoring spin-orbit, decompose D into IRREPs of D_{3d} (the decomposition will be the same as in D'_{3d}). Then decompose the $\mathit{\Gamma}_{S=2}$ spin representation into IRREPs of D_{3d}. Finally, decompose the product $\mathit{\Gamma}_2 \times \mathrm{D} = {}^5\mathrm{D}$ into IRREPs of D_{3d}. You may find the tables in the first appendix to chapter six to be useful.

(c) Starting on the dominant LS coupling end, decompose ${}^5\mathrm{D}$ first into $\mathsf{O}(3)$ IRREPs via addition of angular momentum. Then decompose your result into D'_{3d} IRREPs and show your result agrees with that of part (b).

(d,e,f) Repeat parts (a), (b) and (c) for Cr^{3+}, with electronic configuration $[\mathrm{Ar}]\,3\mathrm{d}^3$, where Hund's first two rules tell us $S = \frac{3}{2}$ and $L = 3$. Now you need to worry about the double group.

Hint : This problem is quite similar to problem 3 on the Spring 2016 exam, the solutions of which are available on the Spring 2018 Homework page. Studying that solution should help you approach this problem, but please note that the group considered in S16 was D_4, which is a proper point group, hence there was no need to evaluate the parity η. D_{3d} is not a proper point group.

Solution :

(a) For Cr^{1+} with electronic configuration $[\mathrm{Ar}]\,3\mathrm{d}^4$, Hund's rules say $S = 2$, $L = 2$, and $J = |L - S| = 0$, so the ground state term is ${}^5\mathrm{D}_0$.

(b) The valence electrons are in the 3d shell, hence $l = 2$ and the parity is $\eta = (+1)^4 = +1$. The spin representation $\mathit{\Gamma}_{S=2}$ is the same as D^+. To decompose a reducible representation $\mathit{\Psi}$, we use the result

$$n_{\mathit{\Gamma}}(\mathit{\Psi}) = \frac{1}{N_G} \sum_{\mathcal{C}} N_{\mathcal{C}}\, \chi^{\mathit{\Gamma}*}(\mathcal{C})\, \chi^{\mathit{\Psi}}(\mathcal{C}) \quad ,$$

which follows from the Great Orthogonality Theorem (see ch. 2 of the Lecture Notes), to determine the number of times a given IRREP $\mathit{\Gamma}$ occurs in the decomposition of $\mathit{\Psi}$. Decomposing $\mathit{\Psi} = \mathrm{D}^+$ into D_{3d} IRREPs, we find $\mathrm{D}^+ = A_{1g} \oplus 2E_g$. Thus,

$$\begin{aligned} \mathit{\Gamma}_2 \times \mathrm{D}^+ &= \big(A_{1g} \oplus 2E_g\big) \times \big(A_{1g} \oplus 2E_g\big) \\ &= A_{1g} \oplus 4E_g \oplus 4E_g \times E_g \\ &= 5A_{1g} \oplus 4A_{2g} \oplus 8E_g \quad . \end{aligned}$$

[1]Remember D_{3d} has 12 elements and D'_{3d} has 24 elements since it is the double group of D_{3d}.

D'_{3d}	E	$3C'_2$	$2C_3$	I	$3\sigma_d$	$2S_6$	$\overline{E}$	$3\overline{C}'_2$	$2\overline{C}_3$	$\overline{I}$	$3\overline{\sigma}_d$	$2\overline{S}_6$
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	−1	1	1	−1	1	1	−1	1	1	−1	1
E_g	2	0	−1	2	0	−1	2	0	−1	2	0	−1
A_{1u}	1	1	1	−1	−1	−1	1	1	1	−1	−1	−1
A_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
E_u	2	0	−1	−2	0	1	2	0	−1	−2	0	1
Θ_g	1	i	−1	1	i	−1	−1	$-i$	1	−1	$-i$	1
Θ_g^*	1	$-i$	−1	1	$-i$	−1	−1	i	1	−1	i	1
Δ_g	2	0	1	2	0	1	−2	0	−1	−2	0	−1
Θ_u	1	i	−1	−1	$-i$	1	−1	$-i$	1	1	i	−1
Θ_u^*	1	$-i$	−1	−1	i	1	−1	i	1	1	$-i$	−1
Δ_u	2	0	1	−2	0	−1	−2	0	−1	2	0	1
P^+	3	−1	0	3	−1	0	3	−1	0	3	−1	0
D^+	5	1	−1	5	1	−1	5	1	−1	5	1	−1
F^+	7	−1	1	7	−1	1	7	−1	1	7	−1	1
G^+	9	1	0	9	1	0	9	1	0	9	1	0
$\Gamma_{1/2}$	2	0	1	2	0	1	−2	0	−1	−2	0	−1
$\Gamma_{3/2}$	4	0	−1	4	0	−1	−4	0	1	−4	0	1
$\Gamma_{5/2}$	6	0	0	6	0	0	−6	0	0	−6	0	0
$\Gamma_{7/2}$	8	0	1	8	0	1	−8	0	−1	−9	0	−1
$\Gamma_{9/2}$	10	0	−1	10	0	−1	−10	0	1	−10	0	1

Table 1: Character table for D'_{3d}, extended to include the last nine representations.

Here we have used $A_{1g} \times \Psi = \Psi$ for any representation Ψ, and $E_g \times E_g = A_{1g} \oplus A_{2g} \oplus E_g$, which is readily derived using the decomposition formula.

(c) Now let's first compute $\Gamma_2 \times \mathrm{D}^+$ in $\mathsf{SO}(3)$. This is easy – just multiply two spin-2 IRREPs to get

$$\Gamma_2 \times \mathrm{D}^+ = \mathrm{S}^+ \oplus \mathrm{P}^+ \oplus \mathrm{D}^+ \oplus \mathrm{F}^+ \oplus \mathrm{G}^+ \quad ,$$

i.e. $2 \times 2 = 0 \oplus 1 \oplus 2 \oplus 3 \oplus 4$. Decomposing these SO(3) IRREPs into IRREPs of D_{3d}, we find

$$\begin{aligned}
\mathrm{S}^+ &= A_{1g} \\
\mathrm{P}^+ &= A_{2g} \oplus E_g \\
\mathrm{D}^+ &= A_{1g} \oplus 2E_g \\
\mathrm{F}^+ &= A_{1g} \oplus 2A_{2g} \oplus 2E_g \\
\mathrm{G}^+ &= 2A_{1g} \oplus A_{2g} \oplus 3E_g \quad .
\end{aligned}$$

Thus we obtain

$$^5\mathrm{D}^+ = \mathit{\Gamma}_2 \times \mathrm{D}^+ = 5A_{1g} \oplus 4A_{2g} \oplus 8E_g \quad ,$$

as in part (a).

(d) Now we come to Cr^{3+}, with electronic configuration [Ar] $3d^4$, Hund's rules tell us that $S = \frac{3}{2}$, $L = 3$, and $J = |L - S| = \frac{3}{2}$, so the ground state term is $^4\mathrm{F}_{3/2}$.

(e) The parity is again $\eta = +1 = (+1)^3$. We first decompose the spin IRREP $\mathit{\Gamma}_{3/2}$. From the entries in the extended character table, obtained Tabs. 6.20 and 6.21 of the Lecture Notes, we find

$$\begin{aligned}
\mathit{\Gamma}_{1/2} &= \Delta_g \\
\mathit{\Gamma}_{3/2} &= \Theta_g \oplus \Theta_g^* \oplus \Delta_g \\
\mathit{\Gamma}_{5/2} &= \Theta_g \oplus \Theta_g^* \oplus 2\Delta_g \\
\mathit{\Gamma}_{7/2} &= \Theta_g \oplus \Theta_g^* \oplus 3\Delta_g \\
\mathit{\Gamma}_{9/2} &= 3\Theta_g \oplus 3\Theta_g^* \oplus 3\Delta_g \quad .
\end{aligned}$$

At the moment, we only need the decomposition of $\mathit{\Gamma}_{3/2}$, as well as that of F^+, which we found in part (c). We therefore have

$$\begin{aligned}
\Gamma_{3/2} \times \mathrm{F}^+ &= \Big(\Theta_g \oplus \Theta_g^* \oplus 2\Delta_g\Big) \times \Big(A_{1g} \oplus 2A_{2g} \oplus 2E_g\Big) \\
&= 5\Theta_g \oplus 5\Theta_g^* \oplus 9\Delta_g \quad ,
\end{aligned}$$

where we use the partial multiplication table Tab. 2, which is easily constructed by multiplying and decomposing D'_{3d} IRREPs. Note that there are $5 + 5 + 9 \cdot 2 = 28 = 4 \cdot 7$ states (4 from $S = \frac{3}{2}$ and 7 from $L = 3$).

(f) Finally, start from the strong LS coupling side, and multiply the SO(3) IRREPs corresponding to $S = \frac{3}{2}$ and $L = 3$. We get

$$\tfrac{3}{2} \times 3 = \tfrac{3}{2} \oplus \tfrac{5}{2} \oplus \tfrac{7}{2} \oplus \tfrac{9}{2} \quad .$$

The decomposition of each of these is given in the solution to part (e). Summing up their decompositions, we once again arrive at

$$^4\mathrm{F}^+_{3/2} = 5\Theta_g \oplus 5\Theta_g^* \oplus 9\Delta_g \quad .$$

D'_{3d}	A_{1g}	A_{2g}	E_g
Θ_g	Θ_g	Θ_g^*	Δ_g
Θ_g^*	Θ_g^*	Θ_g	Δ_g
Δ_g	Δ_g	Δ_g	$\Theta_g \oplus \Theta_g^* \oplus \Delta_g$

Table 2: Products of spin and spinless *gerade* IRREPs of D'_{3d} IRREPs.

[3] The n-string braid group B_n has $(n-1)$ generators $\{\tau_1, \ldots, \tau_{n-1}\}$ obeying the relations

$$\begin{aligned} \tau_i\,\tau_j &= \tau_j\,\tau_i \qquad \text{if } |i-j|>1 \\ \tau_i\,\tau_{i+1}\,\tau_i &= \tau_{i+1}\,\tau_i\,\tau_{i+1} \qquad (1 \le i \le n-2) \quad . \end{aligned}$$

(a) Find all one-dimensional unitary representations of B_n, for all n.

(b) Find all two-dimensional unitary representations of B_3. Recall that a general element $g \in \mathsf{SU}(2)$ may be written as $g = a + ib\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}$, where $a^2 + b^2 = \hat{\boldsymbol{n}}^2 = 1$ and $\boldsymbol{\sigma}$ are the Pauli matrices. Recall also that $\sigma^a\,\sigma^b = \delta^{ab} + i\epsilon_{abc}\,\sigma^c$.

(c) Show that

$$\tau_i = \left[\begin{array}{c|cc|c} \mathbb{I}_{i-1} & 0 & 0 & 0 \\ \hline 0 & 1-t & t & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & \mathbb{I}_{n-i-1} \end{array}\right] \quad , \tag{1}$$

comprises an n-dimensional representation of B_n for any $t \in \mathbb{R}$. This is known as the *Burau representation*. The Burau representation is faithful for $n = 2$ and $n = 3$, but is known to be not faithful for $n \ge 5$. Whether it is faithful for $n = 4$ is an open problem.

Solution :

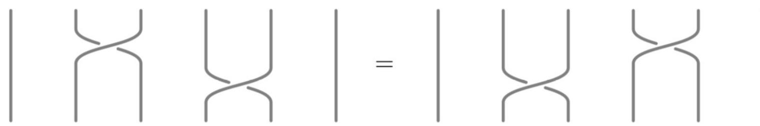
(a) Let $D(B_n)$ be a one-dimensional unitary representation of B_n. It is then commutative, since each element of B_n is represented by a unimodular complex number. From the second of the relations, we have

$$D(\tau_i\,\tau_{i+1}\,\tau_i) = D^2(\tau_i)\,D(\tau_{i+1}) = D(\tau_i)\,D^2(\tau_{i+1}) = D(\tau_{i+1}\,\tau_i\,\tau_{i+1}) \quad .$$

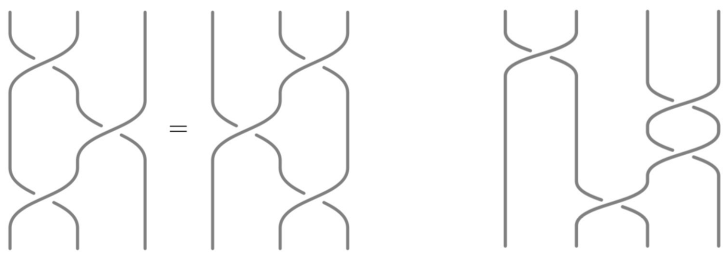
Thus, $D(\tau_i) = D(\tau_{i+1})$ for all $i \in \{1, \ldots, n-2\}$, which means

$$D(\tau_i) = e^{i\theta}$$

for all $i \in \{1, \ldots, n-1\}$, where $\theta \in [0, 2\pi)$.



$\tau_{i+2}\,\tau_i = \tau_i\,\tau_{i+2}$



$\tau_i\,\tau_{i+1}\,\tau_i = \tau_{i+1}\,\tau_i\,\tau_{i+1}$ $\qquad$ $\tau_1\,\tau_3\,\tau_3\,\tau_2$

Figure 1: Braid group relations and construction of a braid group element.

(b) B_3 has two elements, which we call $g = \sigma_1$ and $h = \sigma_2$. We write

$$g = a + ib\,\hat{\boldsymbol{m}}\cdot\boldsymbol{\sigma} \quad , \quad h = c + id\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} \quad ,$$

where $a^2 + b^2 = c^2 + d^2 = \hat{\boldsymbol{m}}^2 = \hat{\boldsymbol{n}}^2 = 1$. There is one group relation, *viz.*

$$ghg = hgh \quad \Longrightarrow \quad ghg^{-1} = h^{-1}gh \quad .$$

This latter form of the relation is convenient since it involves conjugation. Now it is useful to derive the relation

$$(a + ib\,\hat{\boldsymbol{m}}\cdot\boldsymbol{\sigma})(\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma})(a - ib\,\hat{\boldsymbol{m}}\cdot\boldsymbol{\sigma}) = (a^2 - b^2)\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} - 2ab\,\hat{\boldsymbol{m}}\times\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} + 2b^2(\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}})\,\hat{\boldsymbol{m}}\cdot\boldsymbol{\sigma} \quad .$$

From this we derive

$$\begin{aligned} ghg^{-1} &= (a + ib\,\hat{\boldsymbol{m}}\cdot\boldsymbol{\sigma})(c + id\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma})(a - ib\,\hat{\boldsymbol{m}}\cdot\boldsymbol{\sigma}) \\ &= (a^2 + b^2)\,c + id\Big[(a^2 - b^2)\,\hat{\boldsymbol{n}} - 2ab\,\hat{\boldsymbol{m}}\times\hat{\boldsymbol{n}} + 2b^2\,(\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}})\,\hat{\boldsymbol{m}}\Big]\cdot\boldsymbol{\sigma} \end{aligned}$$

and

$$\begin{aligned} h^{-1}gh &= (c - id\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma})(a + ib\,\hat{\boldsymbol{m}}\cdot\boldsymbol{\sigma})(c - id\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}) \\ &= (c^2 + d^2)\,a + ib\Big[(c^2 - d^2)\,\hat{\boldsymbol{m}} - 2cd\,\hat{\boldsymbol{m}}\times\hat{\boldsymbol{n}} + 2d^2\,(\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}})\,\hat{\boldsymbol{n}}\Big]\cdot\boldsymbol{\sigma} \quad . \end{aligned}$$

We may now invoke $a^2 + b^2 = c^2 + d^2 = 1$. Equating these expressions gives $a = c$, and we may also equate the vectors contracted with $\boldsymbol{\sigma}$ in each expression. Taking their dot product with $\hat{\boldsymbol{m}}\times\hat{\boldsymbol{n}}$ gives $abd = bcd$, *i.e.* $(a - c)bd = 0$, which again gives $a = c$. Taking their dot products with $\hat{\boldsymbol{m}}$ and $\hat{\boldsymbol{n}}$, respectively, yields the equations

$$d\,\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}} = b\Big[c^2 - d^2 + 2d^2\,(\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}})^2\Big]$$

and

$$b\,\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}} = d\Big[a^2 - b^2 + 2b^2\,(\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}})^2\Big] \quad .$$

Using $(\hat{\boldsymbol{m}}\times\hat{\boldsymbol{n}})^2 + (\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}})^2 = 1$, we may write these two equations as

$$\begin{aligned} d\,\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}} &= b - 2bd^2\,(\hat{\boldsymbol{m}}\times\hat{\boldsymbol{n}})^2 \\ b\,\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}} &= d - 2db^2\,(\hat{\boldsymbol{m}}\times\hat{\boldsymbol{n}})^2 \quad . \end{aligned}$$

Taken together, these imply $b^2 = d^2$, *i.e.* $d = \pm b$. Thus, we have two possibilities:

(i) $c = a$, $d = +b$, and $\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}} = 1 - 2b^2\,(\hat{\boldsymbol{m}}\times\hat{\boldsymbol{n}})^2$.

(ii) $c = a$, $d = -b$, and $\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}} = 2b^2\,(\hat{\boldsymbol{m}}\times\hat{\boldsymbol{n}})^2 - 1$.

Let us write $\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}} \equiv \cos\alpha$, in which case $(\hat{\boldsymbol{m}}\times\hat{\boldsymbol{n}})^2 = \sin^2\!\alpha$. We then have

$$\sin^2\alpha = 1 - \cos^2\!\alpha = \frac{1 \mp \cos\alpha}{2b^2} \quad ,$$

where the upper sign applies to case (i) and the lower sign to case (ii). In each case, there are two roots, at

$$\cos\alpha = \pm 1 \qquad , \qquad \cos\alpha = \pm\bigg(\frac{1}{2b^2} - 1\bigg) \quad .$$

The second solution requires $b^2 \ge \frac{1}{4}$. We thus have the following possibilities:

(i) $c = a$, $d = b$, $\hat{\boldsymbol{n}} = \hat{\boldsymbol{m}}$ *i.e.* $\cos\alpha = 1$. Then

$$g = h = a + ib\,\hat{\boldsymbol{m}}\cdot\boldsymbol{\sigma} \quad .$$

This representation is abelian. It is equivalent to the case $c = a$, $d = -b$, $\hat{\boldsymbol{n}} = -\hat{\boldsymbol{m}}$ *i.e.* $\cos\alpha = -1$.

(ii) $c = a$, $d = b$ with $b^2 \ge \frac{1}{4}$, and $\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}} = \frac{1}{2b^2} - 1$. Then

$$g = a + ib\,\hat{\boldsymbol{m}}\cdot\boldsymbol{\sigma} \qquad , \qquad h = a + ib\,\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} \quad .$$

This representation is nonabelian. It is equivalent to the case $c = a$, $d = -b$ with $b^2 \ge \frac{1}{4}$, and $\hat{\boldsymbol{m}}\cdot\hat{\boldsymbol{n}} = 1 - \frac{1}{2b^2}$.

(c) Define the matrices

$$A = \begin{pmatrix} 1-t & t & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad , \qquad B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-t & t \\ 0 & 1 & 0 \end{pmatrix} \quad .$$

Then

$$AB = \begin{pmatrix} 1-t & t\,(1-t) & t^2 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

and

$$(AB)A = \begin{pmatrix} 1-t & t\,(1-t) & t^2 \\ 1-t & t & 0 \\ 1 & 0 & 0 \end{pmatrix} = B(AB) \quad .$$

[4] The point groups D_{4d} and D_{6d} are relevant to molecular chemistry, but are not among the 32 crystallographic point groups. Why not? `[50 quatloos extra credit]`

Solution :

D_{4d} contains an eightfold rotation and D_{6d} a twelvefold rotation, neither of which can be a symmetry for any Bravais lattice according to the crystallographic restriction theorem.