Physics 745 - Group Theory

Solutions to Midterm Exam

1. Let us define three more matrices, F, G, and H, defined by

$$F = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad G = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad H = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

The original set is *not* a group, since many of the products are not contained within the group, as we can see in the table at right (for example, row C). If we augment the group with the indicated matrices, it now *is* a group. This can be demonstrated easily, since (1) as shown at right, it satisfies closure, (2) obviously, E is the identity element, (3) as we will demonstrate presently, every element has an inverse, (4) the associative property is a general property of matrices, and need not be specifically demonstrated. In fact, it is easy to see that the matrices represent the actual rotations of a 2D square, which, depending on your nomenclature, is C_{4V} or D_4.

·	*E*	*A*	*B*	*C*	*D*	*F*	*G*	*H*
E	*E*	*A*	*B*	*C*	*D*	*F*	*G*	*H*
A	*A*	*E*	*D*	*F*	*B*	*C*	*H*	*G*
B	*B*	*C*	*E*	*A*	*G*	*H*	*D*	*F*
C	*C*	*B*	*G*	*H*	*E*	*A*	*F*	*D*
D	*D*	*F*	*A*	*E*	*H*	*G*	*B*	*C*
F	*F*	*D*	*H*	*G*	*A*	*E*	*C*	*B*
G	*G*	*H*	*C*	*B*	*F*	*D*	*E*	*A*
H	*H*	*G*	*F*	*D*	*C*	*B*	*A*	*E*

The inverses are the numbers that you multiply to get E. A quick look at the list tells us that everything is its own inverse, except for C and D, which are inverses of each other.

As always, E is in a class by itself, and since H commutes with everything, it must be in a class by itself. It's easy to see, for example, that $B^{-1}CB = D$, so C and D are in the same class. Furthermore, $C^{-1}BC = F$, so B and F go together. Finally, $C^{-1}AC = G$, so A and G go together. The classes are therefore $\{E, H, AG, BF, CD\}$, so there are five classes and five irreducible representations. Four of them have dimension 1, and the last dimension 2.

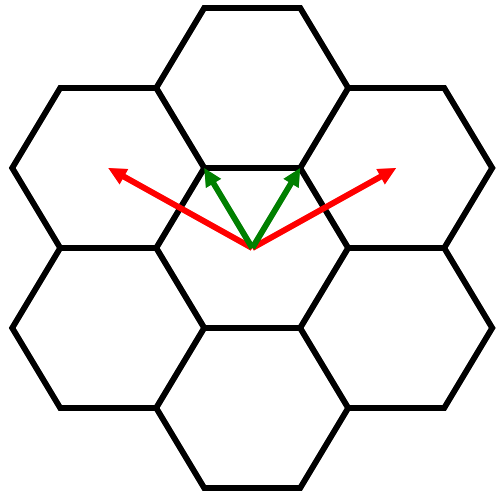
2. The C_2 element was originally a 4-fold rotation axis, so in O_h, it corresponds to C_4^2. The two reflection planes each correspond to JC_4^2, since they can be achieved by performing a 180 degree rotation around some other 4-fold axis of the cube and then performing inversion. And the identity is the identity.

At right is the character table for C_{2V} in the notation of Tinkham, extended a bit to include the O_h irreducible representations. It is not too hard to then work out how the irreps of O_h break up under the reduced symmetry:

C_{2V}	E	C_2	σ_V	σ_V'
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1
Γ_1	1	1	1	1
Γ_2	1	1	1	1
Γ_{12}	2	2	2	2
Γ_{15}'	3	-1	-1	-1
Γ_{25}'	3	-1	-1	-1
Γ_1'	1	1	-1	-1
Γ_2'	1	1	-1	-1
Γ_{12}'	2	2	-2	-2
Γ_{15}	3	-1	1	1
Γ_{25}	3	-1	1	1

$$\Gamma_1 \to A_1,\quad \Gamma_2 \to A_1,\quad \Gamma_{12} \to 2A_1,\quad \Gamma'_{15} \to A_2 \oplus B_1 \oplus B_2,\quad \Gamma'_{25} \to A_2 \oplus B_1 \oplus B_2,$$
$$\Gamma'_1 \to A_2,\quad \Gamma'_2 \to A_2,\quad \Gamma'_{12} \to 2A_2,\quad \Gamma_{15} \to A_1 \oplus B_1 \oplus B_2,\quad \Gamma_{25} \to A_1 \oplus B_1 \oplus B_2$$

3. The point group for this structure is D_{6h}. There is no inherent guarantee that *any* point will have this symmetry, but in this case, the exact center of each hexagon is such a point. The classes associated with this point are:



$$\left\{E, 2C_6, 2C_6^2, C_6^3, 3C'_2, 3C''_2, \sigma_h, 2S_6, 2S_3, J, 3\sigma_V, 3\sigma'_V\right\}$$

There are other ways of writing this as well, equally valid; for example, the second half of this list could be written as J times the first half (I have essentially written it as σ_h times the first half).

The symmetry associated with any carbon atom, on the other hand, is only D_{3h}, since rotations by 60 degrees do not leave the lattice unchanged. The classes are

$$\left\{E, 2C_3, 3C'_2, \sigma_h, 2S_3, 3\sigma_V\right\}.$$

The two red vectors listed are primitive lattice vectors. If the length of the CC bonds is a, these vectors will be

$$\mathbf{T}_1 = a\left(\tfrac{3}{2}\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}\hat{\mathbf{y}}\right),\quad \mathbf{T}_2 = a\left(-\tfrac{3}{2}\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}\hat{\mathbf{y}}\right)$$

There are several other choices about how to draw these vectors.

The reciprocal lattice vectors $\mathbf{G}_1$ and $\mathbf{G}_2$ tend to be perpendicular to $\mathbf{T}_2$ and $\mathbf{T}_1$ respectively; this gives their directions as the green vectors. Their exact values are

$$\mathbf{G}_1 = \frac{2\pi}{a}\left(\tfrac{1}{3}\hat{\mathbf{x}} + \tfrac{1}{\sqrt{3}}\hat{\mathbf{y}}\right),\quad \mathbf{G}_2 = \frac{2\pi}{a}\left(-\tfrac{1}{3}\hat{\mathbf{x}} + \tfrac{1}{\sqrt{3}}\hat{\mathbf{y}}\right)$$

It is then an easy matter to confirm that $\mathbf{T}_a \cdot \mathbf{G}_b = 2\pi\delta_{ab}$, as it should.

The exact form of the structure function will depend on the choice of origin. If it is as marked, then the atoms will be at $\sigma_{c\pm} = \pm\tfrac{1}{3}\left(\mathbf{T}_1 - \mathbf{T}_2\right)$ and $\sigma_{c2} = \tfrac{2}{3}\mathbf{T}_1 + \tfrac{1}{3}\mathbf{T}_2$. If we write our reciprocal lattice vectors as $\mathbf{G} = m_1\mathbf{G}_1 + m_2\mathbf{G}_2$, then $\mathbf{G}\cdot\sigma_{C\pm} = \pm 2\pi\left(m_1 - m_2\right)/3$. As a consequence, our form factor will be

$$S(\Delta\mathbf{k}) = \frac{(2\pi)^2}{\Omega}\sum_{\mathbf{G}}\delta^2\left(\Delta\mathbf{k} - \mathbf{G}\right)\sum_a F_a(\Delta\mathbf{k})\sum_{\boldsymbol{\sigma}_a} e^{i\mathbf{G}\cdot\boldsymbol{\sigma}_a} = \frac{8\pi^2\mathcal{I}(\Delta\mathbf{k})}{3\sqrt{3}a^2}F_C(\Delta\mathbf{k})\sum_{\pm} e^{2\pi i(m_1 - m_2)/3}$$

I have replaced the usual $(2\pi)^3$ by $(2\pi)^2$, representing the fewer number of dimensions, and the "volume" has been replaced by the two dimensional area, since that's all we have here. The imaginary parts of the final sum cancel out, and we end up with

$$S(\Delta\mathbf{k}) = \frac{16\pi^2\mathcal{I}(\Delta\mathbf{k})}{3\sqrt{3}a^2}F_C(\Delta\mathbf{k})\cos\left[\tfrac{2}{3}\pi\left(m_1 - m_2\right)\right]$$

This expression never vanishes, though it is suppressed unless $m_1 - m_2$ is a multiple of three.

4. First note that the states are *always* eigenstates of J as already written, so if we know how they transform under proper rotations, and how they transform under J, the second half of the table will follow automatically from the first half. hence by looking at J alone, we can tell whether we will want the first half of the table given or the second half. The states of the form ψ_{lll} are unchanged under anything that permutes them, as well as anything that changes two of their signs, so in summary, anything with an even number of bars, which are the classes E, C_4^2, C_3, so the relevant matrix must be +1 under each case. The remaining ones will be +1 if l is even, and -1 if l is odd, so the table at right tells you the breakdown.

l	E	$3C_4^2$	$6C_4$	$6C_2$	$8C_3$	J	?
even	1	1	1	1	1	1	Γ_1
odd	1	1	-1	-1	1	-1	Γ'_2

For the states $\psi_{llm}, \psi_{lml}, \psi_{mll}$, we see that under permutations they will transform into each other, which suggests a three-dimensional representation. Under cyclic permutation (C_3), none of them changes into themselves, so the trace will be zero, *i.e.* $\chi(C_3) = 0$. Under C_4^2, one of them is guaranteed to stay the same, while the other two will either change sign (if $m + l$ is odd) or not, so the trace is 3 ($m + l$ even) or -1 ($m + l$ odd). For C_2, you always interchange two of the indices (leaves only one of them the same), then you reverse either the remaining index (+1 if m is even, -1 otherwise) or reverse all three (the same). Hence the result is +1 (m even) or -1 (m odd). For C_4, you interchange a pair of the indices (only one unchanged), then reverse one of the ones you just swapped, giving you +1 (l even) or -1 (l odd). Finally, J reverses all three coordinates, so it is +3 (m even) or -3 (m odd). The corresponding table is at right. Note that when $l + m$ is even, the representation is reducible.

l	m	E	$3C_4^2$	$6C_4$	$6C_2$	$8C_3$	J	?
even	even	3	3	1	1	0	3	$\Gamma_1 + \Gamma_{12}$
even	odd	3	-1	1	-1	0	-3	Γ_{15}
odd	even	3	-1	-1	1	0	3	Γ'_{15}
odd	odd	3	3	-1	-1	0	-3	$\Gamma'_1 + \Gamma'_{12}$

For the six states ψ_{lmn}, there are eight possibilities, but only the number of odd and even indices matters, so this reduces to four cases. The only types of rotations that can have a non-zero character will be those where nothing is permuted, which are E, C_4^2, and J. For C_4^2, we are negating two coordinates at a time, so we get a +2 for each pair of lmn that match parity, and a -2 for each pair of lmn of opposing parity. The result is a total of +6 if lmn are all the same parity, and –2 if lmn contain two of one parity and one of the other parity. As for J, all six wave functions will be +1 if the sum of lmn is even, and all six will be minus if the sum is odd. The table below gives the final results.

l	m	n	E	$3C_4^2$	$6C_4$	$6C_2$	$8C_3$	J	?
even	even	even	6	6	0	0	0	6	$\Gamma_1 + \Gamma_2 + 2\Gamma_{12}$
even	even	odd	6	-2	0	0	0	-6	$\Gamma_{15} + \Gamma_{25}$
even	odd	odd	6	-2	0	0	0	6	$\Gamma'_{15} + \Gamma'_{25}$
odd	odd	odd	6	6	0	0	0	-6	$\Gamma'_1 + \Gamma'_2 + 2\Gamma'_{12}$