Reminder: Group Theory

Let's get some help with computers. What are the groups of order $|G| = 400$? Here is the computer program.[1]

```
G := AllSmallGroups(400);;
List(G, g -> StructureDescription(g));
[ "C25 : C16", "C400", "C25 : C16", "C25 : Q16", "C8 x D50",
  "C25 : (C8 : C2)", "C25 : QD16", "D400", "C2 x (C25 : C8)",
  "C25 : (C8 : C2)", "C4 x (C25 : C4)", "C25 : (C4 : C4)",
  "C25 : (C4 : C4)", "C25 : ((C4 x C2) : C2)", "C25 : QD16", "C25 : D1
  "C25 : Q16", "C25 : QD16", "C25 : ((C4 x C2) : C2)", "C100 x C4",
  "C25 x ((C4 x C2) : C2)", "C25 x (C4 : C4)", "C200 x C2",
  "C25 x (C8 : C2)", "C25 x D16", "C25 x QD16", "C25 x Q16",
  "C25 : (C8 x C2)", "C25 : (C8 : C2)", "C4 x (C25 : C4)",
  "C25 : (C4 : C4)", "C2 x (C25 : C8)", "C25 : (C8 : C2)",
  "C25 : ((C4 x C2) : C2)", "C2 x (C25 : Q8)", "C2 x C4 x D50",
  "C2 x D200", "C25 : ((C4 x C2) : C2)", "D8 x D50",
  "C25 : ((C4 x C2) : C2)", "Q8 x D50", "C25 : ((C4 x C2) : C2)",
  ...
]
```

Notice there is is both $C_{25} \times QD_{16}$ and $C_{25} \ltimes QD_{16}$.

In more commom notation we can write with the symbols $\times$ (direct product) and $\ltimes$ (indirect product):

- $G = (C_5 \ltimes Q_8) \times D_{10}$
- $G = (C_5 \ltimes C_5) \ltimes (C_4 \times C_4)$
- $G = C_2 \times ((C_5 \times C_5) \ltimes C_8)$
- $G = D_8 \times ((C_5 \times C_5) \ltimes C_2)$

Once we have these explicit descriptions of groups, we look at the representation theory of finite groups. Example, by linear algebra:

$$\dim \mathrm{Ind}_H^G(\mathbf{1}_H) = [G : H] = \dim(V)$$

[1] https://math.stackexchange.com/questions/4108993/the-221-groups-of-order-g-400
https://www.gap-system.org/

At least theoretically we can relate the induced representation from the subgroups and the character theory of the subgroups.

$$\sum_{\rho} (\dim \rho)^2 = |G|$$

This is called **Maschke's Theorem**. We have 500 examples to check dimensions of representation and Harmonic analysis of finite groups.[2]

[2] The category is called Mod_G so that functorial properties there could be related to character theoretic formulas here.

Approximate Groups Does "commutativity" matter? We've been studying the equation $ab = ba$. It certainly works for numbers $2 \times 3 = 3 \times 2$ and we can describe when it fails:

$$\left[\begin{array}{cc} 1 & 1 \\ 0 & 1 \end{array} \right] \left[\begin{array}{cc} 1 & 1 \\ 1 & 0 \end{array} \right] = \left[\begin{array}{cc} 2 & 1 \\ 1 & 0 \end{array} \right] \neq \left[\begin{array}{cc} 1 & 2 \\ 1 & 0 \end{array} \right] = \left[\begin{array}{cc} 1 & 1 \\ 1 & 0 \end{array} \right] \left[\begin{array}{cc} 1 & 1 \\ 0 & 1 \end{array} \right]$$

so we have lots of examples of non-commutativity.

Lemma Let G be an aribtary group. Let $A \subset G$ be a subset with $|A^2| \leq K|A|$. Then $|A^{-1}A| \leq K^2|A|$ and $|AA^{-1}| \leq K^2 A$.

In my experience the proofs not very exciting. Counting he possibilities on both sides and making sure both sides are equal. Here's the counter-example the book has provided: Let H be a finite group and $G = H * \langle x \rangle$, the free-product of H and the infinite cyclic group one generatory (basically $\mathbb{Z}$). Set $A = H \cup \{x\}$. Then

$$|A^2 \leq 3|A| \tag{$*$}$$

but $HxH \subseteq A^3$ and yet $|HxH| = |H|^2 \asymp |A|^2$.

This is their instance of **small tripling**. We could imamgine $A \subseteq \mathbb{Z}$ then:

$$A = A + A + A \text{ or } |3A| \leq 3|A|$$

so once we throw away the exact relation $A + A = A$ (such as the arithmetic progression or a **subgroup** or **coset** of $\mathbb{Z}$) we get to consider small-doubling or small-tripliing moves.

Ex $(A \cup \{1\} \cup A^{-1})^2$ is an $O(K^9)$-approximate group.

representation theory[3] Just a reminder that $\int$ is just a short-hand of $\sum$ which just means "$+$".

$$\int_G f(xg)\,d\mu(x) = \int_G f(x)d\mu(x)$$

we need Haar measure on group of choice $G = \mathbb{R}/\mathbb{Z}$ or $G = \mathbb{R}^d$ or (non-abelian) $G = \mathsf{SO}(3)$ (the space of rotations of the sphere). We could get the approximate-groups by setting $f = 1_A$!

? Where did we get these invariant measures and perfect lattices and spheres?

Thm (Peter-Weyl) Let G be a compact topological group with Haar measure μ. Then the regular representation of G on the space $L^2(G,\mu)$ decomposes to Hilbert spae direct sum:

$$L^2(G,\mu) = \bigoplus_{\rho} M(\rho)$$

of isotypic components of the finite dimensional unitary representations, each $M(\rho)$ being isomorphic to $\dim(\rho)$ copies of ρ.

Q What does it measn that $\mathsf{SO}(3)$ is a **compact** topological group?

[3] `https://people.math.ethz.ch/~kowalski/representation-theory.pdf`

05/03 Here's the discussion of Group Theory in the Quantum Chemistry textbook. Here the group is called $\mathcal{C}_{3v}$:

R	Γ^1	Γ^2
E	1	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
C_2	1	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$
C_2^2	1	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$
σ	1	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
σ'	1	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$
σ''	1	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$

These "representations" have to with "function spaces" the d-orbital in Chemistry. For example, the electron iron is written Fe $=$ [Ar] $3d^6\,4s^2$.

"Reducible" representation means the matrix can be diagonalized in two parts:

$$D(R) = \begin{bmatrix} D^1(R) & [0] \\ \\ [0] & D^2(R) \end{bmatrix}$$

The representations E and σ are reducible and could be written as 1×1 matrices instead of 2×2 matries. There are also **4** copies of the same representation.

The d orbital wave functions exist as functions in 3D space and yet this is the symmetry group of a triangle. $\Gamma = \Gamma^1 \oplus 2\Gamma^2$ and $|G| = 6 = 1 \times 1 + 2 \times 2$. That would be interesting if we cound the representation *first* and decided which group it corresponded to. Or we could imagine various representations of the same group and we have to decide if they're "the same".

Notes on Hilbert Space The wave functions are functions $f : S^2 \to \mathbb{R}$.

$$(f_1, f_2) = \int_S^2 f_1^* f_2 \, d\tau = \delta_{ij}$$

We can "rotate" the integral, as well as the "functions" of our atom:

$$(O_R f_i, O_R f_j) = \int (O_R f_i)^* (O_R f_j) d\tau = (f_i f_j) = \delta_{ij}$$

These integral calculations all live in the Hilbert space $L^2(S^2)$:

$$\begin{aligned} \frac{4}{3}\pi a^3 \overline{z} &= \int_0^r \int_{-1}^1 \int_0^{2\pi} r^3 \mu dr \mu d\theta \\ &= \frac{1}{4} \int_{-1}^1 \int_0^{2\pi} a^4 + 4^3 a^3 \alpha (\sum a_n Y_n) d\mu d\theta \\ &= 4a^3 \alpha a_1 \int_{-1}^1 \int_0^{2\pi} \mu Y_1 d\mu d\theta \end{aligned}$$

We might even recognize the volume formula for the sphere $V = \frac{4}{3}\pi a^3$. These are formulas for deducing the **center of gravity** of a nearly spherical object.

- $\frac{4}{3}\pi a^3 \overline{x} = 4a^3 \alpha \cdot a_1 \int_{-1}^1 \int_0^{2\pi} \sqrt{1-\mu^2} \cos\theta Y_1 d\mu d\theta$
- $\frac{4}{3}\pi a^3 \overline{x} = 4a^3 \alpha \cdot a_1 \int_{-1}^1 \int_0^{2\pi} \sqrt{1-\mu^2} \cos\theta Y_1 d\mu d\theta$

It seems the spherical harmonic are necessary for when the shape is not a perfect shere. We still use elements that are symmetric under the varous groups.

References

[1] https://en.wikipedia.org/wiki/Iron
https://en.wikipedia.org/wiki/Block_(periodic_table)#d-block