Universität Tübingen, Mathematisches Institut Sommersemester 2021
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Groups and Representations

Instruction 8 for the preparation of the lecture on 17 May 2021

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3 Applications in quantum mechanics

3.1 Expansion in irreducible basis functions and selections rules

Setting:

L^2-spaces & unitary operators https://youtu.be/5yJbnMbWZK4 (2 min) (1)

Lemma 8. *Let G be a (finite) group of unitary linear operators $V \to V$, $A \in G$,*[1] *and let $\psi_1^\nu, \dots, \psi_{d_\nu}^\nu$ be functions that transform in the unitary irreducible representation Γ^ν (with $\dim(\Gamma^\nu) = d_\nu$), i.e.*

$$A\psi_\alpha^\nu = \sum_{\beta=1}^{d_\nu} \psi_\beta^\nu \, \Gamma^\nu(A)_{\beta\alpha} \, .$$

Then $\exists\, C_\nu \in \mathbb{C}$ such that $\langle \psi_\alpha^\nu | \psi_\beta^\mu \rangle = C_\nu \, \delta_{\nu\mu} \, \delta_{\alpha\beta}$.

Proof:

https://youtu.be/Ru30m0wiOTM (7 min) (2)

Remarks:

https://youtu.be/i-KGixakDDM (3 min) (3)

Have you heard the term *selection rule* before? If not, never mind. If yes, in which context? Let's speak about it in the live session.

3.2 Invariance of the Hamiltonian and degeneracies

A special role is played by the *Hamiltonian* $H : V \to V$ (a linear self-adjoint operator) of a quantum mechanical system. In particular, its eigenvalues are the possible *energy levels* in which we can find the system.

Let H be the Hamiltonian of a quantum mechanical system and let A be a unitary operator. If

$$AH = HA \, ,$$

we say that A commutes with the Hamiltonian or that A *leaves H invariant.*

The set of all symmetry operations (realised by unitary operators) that leave H invariant forms a group G, the *symmetry group* of H. **Why is this a group?**

Every eigenspace of H, say $\{\psi \in V : H\psi = E\psi\}$, carries a representation of the symmetry group G:

https://youtu.be/t0_HAXTVgmg (2 min) (4)

[1] Alternatively, view the operators A as unitary representation of a group G on V.

This representation can, in principle, be reducible or irreducible; typically it is irreducible:

- All states transforming in the same irrep of G must have the same energy:

https://youtu.be/hdODKxaR4Ec (3 min) (5)

- States transforming in different irreps can have different energies – at least, symmetry does not force them to have the same energy:

https://youtu.be/er1ZQ3a8_38 (2 min) (6)

If states transforming in different irreps still have the same energy, we speak about "accidental degeneracy". Possible reasons:

- "Fine-tuning" of one or several parameters in H (unlikely).
- We haven't correctly identified the full symmetry group, i.e. we have overlooked some symmetry.

Conclusions:

- Degenerate states to a given energy typically transform in an irrep of the symmetry group of H, i.e. they can be classified by irreps.
- number of degenerate states = dimension of the irrep

Example (& outlook): Hydrogen atom

https://youtu.be/fYfsXfVIh3E (8 min) (7)