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Quantum Mechanics (See the Tinkham book.)

In Quantum Mechanics we define the physics of a system by giving the Hamiltonian. For example, the hydrogen atom (electron and proton at the origin):

$$H = \frac{\boldsymbol{p}^2}{2m} + V(r), \quad \text{in this case with } V(r) = -\frac{e^2}{r} = -\frac{e^2}{\sqrt{x^2+y^2+z^2}}.$$

This leads to the Schrödinger equation (time-independent):

$$\hat{H}\psi_n(\boldsymbol{r}) = E_n \psi(\boldsymbol{r})$$

with $\boldsymbol{r} = (x, y, z)$ and $\hat{H}$ is the quantised Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

E_n is the eigenvalue of ψ_n. The symmetry is O(3) (more later today). To relate to finite groups we consider instead a 3-proton situation ("molecular").

Figure 1. Three protons, and an electron moving around in the potential created by them.

The electron in the field from these three protons moves in a complicated potential. *But* without solving the problem explicitly we can say quite a lot about the problem using the finite group D_3 which is the symmetry group of the three proton "molecule".

Introduce an operator $\hat{P}_R$ corresponding to some symmetry operation of the triangle. Being a symmetry operation we must have

$$\hat{P}_R \hat{H} = \hat{H}\hat{P}_R,$$

i.e. $\hat{P}_R$ commutes with $\hat{H}$.

$$\hat{H}\Big(\hat{P}_R\psi_n\Big) = E_n\Big(\hat{P}_R\psi_n\Big)$$

So $\hat{P}_R\psi_n$ is a new wave function with the same eigenvalue as ψ_n.

Recalling the Wigner definition of $\hat{P}_R$:

$$\hat{P}_R\psi_n(\boldsymbol{r}) \equiv \psi_n\big(R^{-1}(\boldsymbol{r})\big)$$

(i.e. $\hat{P}_R\psi(R(\boldsymbol{r})) = \psi(\boldsymbol{r})$). Compare $\boldsymbol{r} = x\,\boldsymbol{e}_x + y\,\boldsymbol{e}_y + z\,\boldsymbol{e}_z$ or to quantum mechanics: $\psi(\boldsymbol{r}) = \langle \boldsymbol{r}|\psi\rangle$. $1 = R^{-1}R$.

This means that the eigenfunctions ($\psi_n(\boldsymbol{r})$'s) group themselves into irreducible representations of D_3.

$$\hat{P}_R\psi_n^{(i)} = \sum_m \psi_m^{(i)}\Big(\Gamma^{(i)}(R)\Big)_{mn}$$

where (i) denotes one particular irreducible representation, and these l_i (dimension of the irreducible representation) wave functions all have eigenvalue E_n.

The *normal* situation then is that different irreducible representations have different eigenvalues. If not there is an *accidental degeneracy*.

Example: In the hydrogen atom the 2s and 2p states are degenerate. This degeneracy is lifted for *hydrogen-like* atoms.

Example: The cyclic group, C_h, of order h has elements $\{E, A, A^2, ..., A^{h-1}\}$ such that $A^h = E$. It is generated by one element A. These groups are *abelian* $\Rightarrow$ each element gives a conjugacy class $\Rightarrow$ there are h conjugacy classes and thus h different irreducible representations $\Rightarrow$ all the irreducible representations are one-dimensional:

$$\sum_{i=1}^{h} (l_i)^2 = h \quad \Rightarrow \quad \text{all } l_i = 1$$

$$\Rightarrow \Gamma^{(i)} = \mathrm{e}^{2\pi \mathrm{i} r/h}, \quad r = 0, 1, ..., h-1, \quad \left(\Gamma^{(i)}\right)^h = 1$$

This implies *Bloch's theorem in solid state*:

Consider an electron in a one-dimensional periodic lattice with period $L = a \cdot h$ where a is the lattice spacing and h is the number of lattice sites.

$$\Rightarrow \quad \hat{P}_a \psi^{(r)}(x) = \psi^{(r)}(x+a) \underset{\text{lattice}}{\overset{\text{cyclic}}{=\!=}} \psi^{(r)}(x)\, \mathrm{e}^{2\pi \mathrm{i} r/h}$$

$\hat{P}_a$ is the translation operator, distance a. h steps goes back to origin.

$$\Rightarrow \quad \psi^{(r)}(x+a) = [L = a\, h] = \mathrm{e}^{2\pi \mathrm{i} r a/L}\, \psi^{(r)}(x) = [k = 2\pi r/L] = \mathrm{e}^{\mathrm{i} k a} \psi^{(r)}(x)$$

This equation has the general solution:

$$\psi_k(x) = u_k(x)\, \mathrm{e}^{i k x}$$

where $u_k(x)$ is periodic with perid a. This is Bloch's wave function.

Chapter 3 Continuous groups.

Recall the Schrödinger equation

$$\hat{H} \psi_n(\boldsymbol{r}) = E_n \psi_n(\boldsymbol{r})$$

This is rotationally invariant, i.e. has symmetry O(3):

$$\boldsymbol{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \quad \boldsymbol{r} \rightarrow \boldsymbol{r}' = R\, \boldsymbol{r}, \quad \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} R_{xx} & R_{xy} & \cdots \\ R_{yx} & \cdots & \\ R_{zx} & \cdots & \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

or $x_i \rightarrow x_i' = \sum_j R_{ij} x_j$, $i = 1, 2, 3$. Using Einstein's summation convention: $x_i' = R_{ij} x_j$. Scalar product $r^2 = |\boldsymbol{r}|^2 = \boldsymbol{r}^T \boldsymbol{r} = x_i x_i = \begin{pmatrix} x & y & z \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$. Rotational invariance of r^2 means

$$(r')^2 = r^2$$

$$\Rightarrow (r')^2 = \boldsymbol{r}^T R^T R\, \boldsymbol{r} = \boldsymbol{r}^T \boldsymbol{r}$$

Invariance implies $R^T R = \mathbf{1} \Leftrightarrow R \in \mathrm{O}(3)$, the orthogonal group in three dimensions. (Exercise: check group axioms.)

Note:

$$\left(R^T\right)_{ij}(R)_{jk}=\delta_{ik}$$

(sum over j implied)

$$(R)_{ji}R_{jk}=\delta_{ik}$$

(sum over j)

Now for $i=k$ (no sum)

$$\sum_j (R_{ij})^2=1$$

$$|R_{ij}|\leqslant 1$$

All matrix elements in R are bounded by 1; i.e., the group is compact. So R can be expressed in terms of angles. How many angles? n dimensions, $\mathrm{O}(n)$. R has n^2 elements and $R^TR=1$ gives $n\,(n+1)/2$ equations (since a symmetric equation).

R has $n^2-n(n+1)/2=n(n-1)/2$ elements.

Example: $n=3$, number $=3$. $n=4$, number $=6$.

The invariance of r^2 (and hence the group $\mathrm{O}(n)$) can be described in terms of a *tensor* δ_{ij}. So invariance of r^2 is equivalent to δ_{ij} being an *invariant tensor*.

Introduce covariant and contravariant indices: x^i (covariant index) and x_i (contravariant index). Then we use as a definition (or input information) that $x^i\xrightarrow{R}x'^{\,i}=x^jR_j{}^i$. The position of indices is important. Then

$$x_i\xrightarrow{R}x'_i=\left(R^{-1}\right)_i{}^jx_j$$

In other words x^ix_i is invariant without any restrictions on R. Any *tensor* $T_{ijk}{}^{lmnpq}$ will now rotate according to these rules.

$$T_{ij}{}^k\rightarrow T'_{ij}{}^k=\left(R^{-1}\right)_i{}^{i'}\left(R^{-1}\right)_j{}^{j'}T_{i'j'}{}^{k'}R_{k'}{}^k$$

So this x^ix_i is *not* a scalar product. It relates properties of dual vector spaces. Scalar products then relates to x in the same space:

$$r^2=x^i\delta_{ij}x^j$$

So in general (any R) will transform this δ_{ij} to

$$\delta'_{ij}=\left(R^{-1}\right)_i{}^{i'}\left(R^{-1}\right)_j{}^{j'}\delta_{i'j'}$$

but for $R\in\mathrm{O}(3)$ we get $\delta'_{ij}=\delta_{ij}$, i.e. δ_{ij} is an $\mathrm{O}(3)$-invariant tensor.

Normally this is written

$$R_i{}^{i'}R_j{}^{j'}\delta_{i'j'}=\delta_{ij}$$

or in matrix notation

$$R\,\mathbf{1}\,R^T=\mathbf{1}\quad\Rightarrow\quad R\,R^T=\mathbf{1}$$

Another example is from quantum mechanics. The wave function of a spin $\frac{1}{2}$ part is

$$\chi = \begin{pmatrix} \chi_1(\boldsymbol{r}) \\ \chi_2(\boldsymbol{r}) \end{pmatrix}, \quad \chi_i \in \mathbb{C}$$

and "scalar" in quantum mechanics is $\chi^\dagger \chi$. Call these components z_i instead:

$$\boldsymbol{z}^\dagger \boldsymbol{z} = \begin{pmatrix} z_1^* & z_2^* \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = |z_1|^2 + |z_2|^2$$

What is the invariant group?

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \rightarrow \begin{pmatrix} z_1' \\ z_2' \end{pmatrix} = U \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$$

where U is a 2×2 complex matrix.

$$U^\dagger U = 1 \quad \Leftrightarrow \quad U \in \mathrm{U}(2)$$

and in $z_i \in \mathbb{C}^n$: $U \in \mathrm{U}(n)$.

Note: $R \in \mathrm{O}(3)$ then $R^T R = 1$. Take the determinant, and we have $(\det R)^2 = 1 \Rightarrow \det R = \pm 1$ and we define $R \in \mathrm{SO}(3)$ if $\det R = +1$. (This property is conserved by matrix multiplication). $\tilde{R}$ with $\det \tilde{R} = -1$ does not give a group.

So O(3) has two *components* (a *component* is the set of matrices R continuously related to each other).

OBS. Both O(3) and SO(3) has three continuous parameters.

Note: $U \in \mathrm{U}(2)$ then $U^\dagger U = \mathbf{1} \Rightarrow \det U^* \det U = 1 \Rightarrow \det U = \mathrm{e}^{\mathrm{i}\alpha}$. By defining SU(2) by $\det U = +1$ we see that $\mathrm{U}(2) = \mathrm{U}(1) \times \mathrm{SU}(2)$. U(1) is the phase $\{\mathrm{e}^{\mathrm{i}\alpha}\}$. Going from U(2) to SU(2) eliminates one continuous parameter, unlike the case with O(3) $\leftrightarrow$ SO(3).

Recall: $U \in \mathrm{SU}(2)$ can be written as

$$U = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}$$

Check $U^\dagger U = 1, \det U = 1 \Rightarrow |a|^2 + |b|^2 = 1. \ \sim S^3$.

Example. Newtonian mechanics. It is *invariant* under O(3) and translations in (x, y, z, t) meaning that Newton's equations are *covariant*.

This is the *Galilei* group: this is a semi-direct product of the O(3) and translation group. The translation group is abelian. Writing $(R, \boldsymbol{a})$ with $R \in \mathrm{O}(3)$ and $\boldsymbol{a}$ being the translation ($\boldsymbol{r} \rightarrow \boldsymbol{r} + \boldsymbol{a}$) then

$$(R, \boldsymbol{a}) \times (S, \boldsymbol{b}) = (R S, R \boldsymbol{b} + \boldsymbol{a})$$

This implies that $\mathrm{Gal} = \mathrm{O}(3) \ltimes$ translation. (Neglecting time.)

Exercise: Show that this rule satisfies the group axioms.

Exercise: Show that rule follows from

$$(R, \boldsymbol{a}) \Leftrightarrow \left(\begin{array}{c|c} R & \boldsymbol{a} \\ \hline \mathbf{0} & 1 \end{array}\right)$$

Example: Special relativity:

Defined by the invariant tensor

$$\eta_{\mu\nu} = \begin{pmatrix} -1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & 1 \end{pmatrix}$$

If $\Lambda \in \mathrm{SO}(1,3)$ then $\Lambda_\mu{}^\rho \, \Lambda_\nu{}^\sigma \, \eta_{\rho\sigma} = \eta_{\mu\nu}$ or as matrices $\Lambda \, \eta \, \Lambda^T = \eta$.

Note: The covariant and contravariant indices are related by the inverse metric tensor:

$$x^\mu = \eta^{\mu\nu} x_\nu$$

One can obtain $\Lambda \eta \Lambda^T = \eta$ from comparing the transformation rules of x^μ and x_μ. (Excercise.)

Example: General relativity:

Here the *only* invariant tensor is the volume tensor $\varepsilon^{\mu\nu\rho\sigma}$ and the group is $\mathrm{Diff}(M)$ – diffeomorphisms of the manifold – the set of all coordinate transformations. Multiplication rule = composition of maps.

$$x^\mu \xrightarrow{f_1} \tilde{x}^\mu = \tilde{x}^\mu(x) \xrightarrow{f_2} \tilde{\tilde{x}}^\mu = \tilde{\tilde{x}}^\mu(\tilde{x}) = \tilde{\tilde{x}}^\mu(\tilde{x}(x))$$

of $f_2 \circ f_1 = f_3$. In general relativity we use $\partial_\mu = \frac{\partial}{\partial x^\mu}$ and $\mathrm{d}x^\mu$ as protoptypes for contravariant and covariant tensors.

Chain rule:

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = \frac{\partial \tilde{x}^\nu}{\partial x^\mu} \frac{\partial}{\partial \tilde{x}^\nu}$$

also

$$\mathrm{d}\tilde{x}^\mu = \frac{\mathrm{d}\tilde{x}^\mu}{\partial x^\nu} \mathrm{d}x^\nu$$

Then the vector fields $V \equiv V^\mu \partial_\mu$ and diff 1-forms $\omega = \mathrm{d}x^\mu \omega_\mu$ are invariant under $\mathrm{Diff}(M) \Rightarrow$ transformation rules for V^μ and ω_μ.

Note: exterior differential $\mathrm{d} = \mathrm{d}x^\mu \, \partial_\mu$ is autmatically coordinate invariant.

Note: it is possible to introduce special invariant tensors $\Rightarrow$ "structures".