## 2012–02–07 

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**Quantum Mechanics** (this part is basically from the book by Tinkham)

In Quantum Mechanics we often define the physics by a Hamiltonian (energy).

Example: Hydrogen atom.

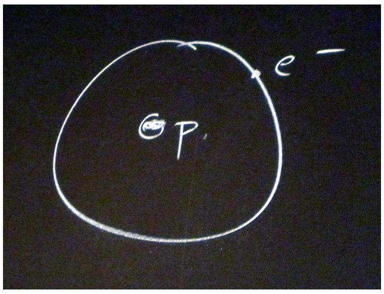


**Figure 1.** Hydrogen atom: an electron orbiting a proton.

$$H = \frac{p^2}{2m} + V(r) \quad \text{where} \quad V(r) = -\frac{e^2}{r}.$$

$H$ is invariant under rotations: SO(3).

$H$ gives the Schrödinger equation.

$$\hat{H}\psi_n = E_n\psi_n$$

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

Here the symmetry is SO(3), which is the continous rotations in three dimensions. But from the point of view of discrete groups we could imagine the electron move in the field of three sources in a triangle (figure 2). This means that SO(3) is replaced by $D_3$.

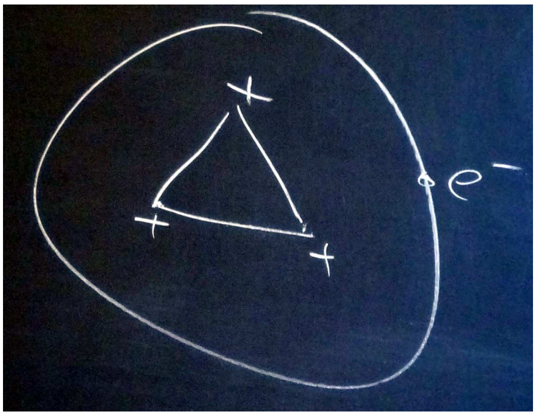


**Figure 2.** An electron moving around a symmetric triatomic molecule.

In any of these cases this means, with $\hat{P}_R$ being a symmetry operation (i.e. an element of the symmetry group), that $\hat{P}_R\hat{H} = \hat{H}\hat{P}_R$. The symmetry operation must commute with the Hamiltonian.

$$\hat{H}(P_R\psi_n) = E_n(P_R\psi_n)$$

i.e. if $\psi_n$ is a solution the Schrödinger equation, so is $P_R\,\psi_n$, and with the same eigenvalue. So a symmetry leads to degenerate eigenvalues and the total set of degenerate eigenfunctions must constitute a representation of the symmetry group.

Then we define (Wigner)

$$\hat{P}_R\,\psi_n(x,y,z) = \ldots$$

$\hat{P}_R$ changes the function $\psi$. $R$ is actually a rotation, either continuous or discrete. Then we define

$$\hat{P}_R\,\psi_n(x,y,z) = \psi_n(R^{-1}(x,y,z))$$

Note that we get the inverse $R^{-1}$ here.

If $(i)$ (the representation index) and $a, b$ enumerate the degenerate $\psi$'s: For each eigenvalue $E_n$

$$\hat{P}_R\,\psi_a^{(i)} = \sum_{b=1}^{l_i} \psi_b^{(i)}\big(\Gamma^{(i)}(R)\big)_{ba}$$

Let's do Bloch's theorem now.

Example: Bloch's theorem: We have an electron moving in a lattice in one dimension. Lattice we assume to be periodic with lattice spacing $a$, number of sites $h$ and the length is $L = a\,h$. We identify the end points so that it is rather like a circle (figure 3).

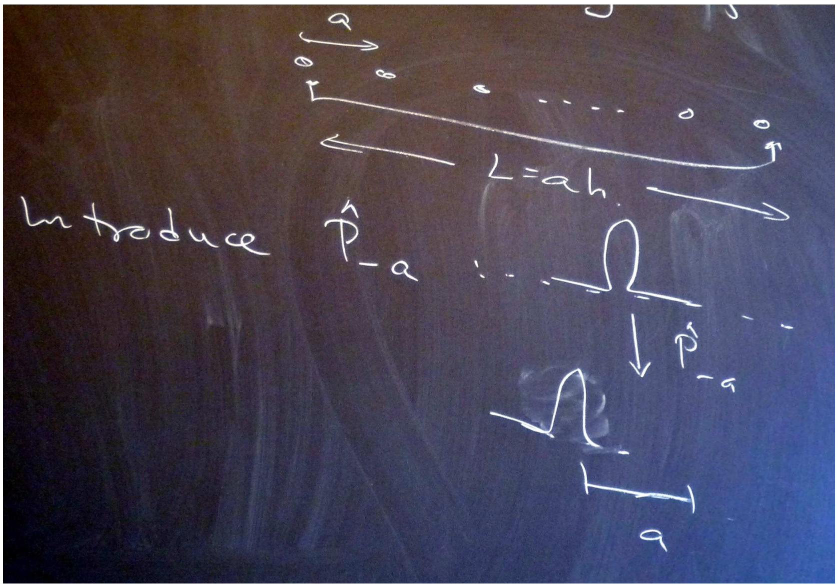


**Figure 3.**

Introduce the operator $\hat{P}_{-a}$ (figure 3), shifting the function to the left.

$$\Rightarrow \hat{P}_{-a}\psi^{(r)}(x) = \psi^{(r)}(P_{-a}^{-1}(x)) = \psi^{(r)}(x+a)$$

$(r)$ is representation label.

The group acting on the lattice is cyclic group $Z_h$, with $\big(\hat{P}_a\big)^h = \hat{P}_{\text{identity}}$. Representations are one-dimensional complex: $\mathrm{e}^{2\pi\mathrm{i}r/h}$.

$$\Rightarrow \quad \hat{P}_{-a}\psi^{(r)}(x) = \psi^{(r)}(x+a) = \psi^{(r)}(x)\,\mathrm{e}^{2\pi\mathrm{i}r/h}$$

$$\psi^{(r)}(x+a) = \mathrm{e}^{2\pi\mathrm{i}ra/L}\psi^{(r)}(x) \equiv \mathrm{e}^{\mathrm{i}ka}\psi^{(r)}(x)$$

where $k = 2\pi r/L$. So, now denote the representation by $k$ instead of $r$ (as is standard)

$$\Rightarrow \psi_k(x+a) = \mathrm{e}^{\mathrm{i}ka}\psi_k(x)$$

Bloch's theorem says that the general solution to this equation is

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

where $u_k(x)$ is periodic with period $a$.

**Direct and semi-direct product groups.**

Suppose we have a group $G$ which has two normal (or invariant, that's the same thing) subgroups $H_1$ and $H_2$. Then we can form $G/H_1$ and $G/H_2$ and they will both be groups, and hence

$$G = G/H_1 \times H_1 = G/H_2 \times H_2$$

1. If $G/H_1 = H_2$ and $G/H_2 = H_1$ then $G$ is the direct product of $H_1$ and $H_2$, written

$$G = H_1 \times H_2.$$

2. Consider now $D_3$. It has two subgroups, $A_3$ and $D_2$. One is a normal subgroup and the other is not. $A_3$ is normal — if you conjugate $A_3$ with all the elements of $D_3$ you get back $A_3$.

$$D_3 = \{E, A, B, C, D, F\}$$

$$A_3 = \{E, D, F\}: \quad \text{rotations}$$

$$D_2^{(A)} = \{E, A\}, \quad D_2^{(B)} = \{E, B\}, \quad D_2^{(C)} = \{E, C\}.$$

The conjugation of the $D_2$'s will mix them (using $A_3$ when conjugating the elements). $A_3$ acts on the $D_2$.

$$D_3 = A_3 \rtimes D_2$$

$A_3$ normal, $D_2$ not normal. This is called the *semi-direct product*.

Example: Poincaré group $(\Lambda,\ T)$ where $\Lambda$ are rotations in space-time (homogeneous Lorentz transformations), and $T$ are translations.

$$(\Lambda_1, T_1)(\Lambda_2, T_2) = (\Lambda_1\Lambda_2, \Lambda_1 T_2 + T_1)$$

Easy to see by writing

$$\begin{pmatrix} \Lambda & T \\ 0 & 1 \end{pmatrix}$$

Exercise!

*Note:* Matrices for $G = H_1 \times H_2$ are

$$\underbrace{\Gamma_{AB}^{(G)}}_{\in G} = \underbrace{\Gamma_{ab}^{(H_1)}}_{\in H_1}\underbrace{\Gamma_{\alpha\beta}^{(H_2)}}_{\in H_2}$$

We can view the $A$ and $B$ as composite indices: $A = (a, \alpha), B = (b, \beta)$.

$$\Rightarrow \sum_I (l_I)^2 = \sum_{ij} \left(l_i^{(1)}\, l_j^{(2)}\right)^2 = \sum_i \left(l_i^{(1)}\right)^2 \sum_j \left(l_j^{(2)}\right)^2 = h^{(1)}\, h^{(2)} = g$$

Now we have a break.

**Chapter 3: Continuous groups = Lie groups**

EXAMPLE

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

where $V(r)$ is a *central* potential, that only depends on $r = \sqrt{x^2 + y^2 + z^2}$, and $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$ where $\partial_x \equiv \frac{\partial}{\partial x}$. This all means that $\hat{H}$ is SO(3) invariant, where SO(3) is the group of three-dimensional rotations.

*So:* Rotations in three dimensions. We take a vector $\boldsymbol{r}$ and we rotate it:

$$\boldsymbol{r} \to \boldsymbol{r}' = R\,\boldsymbol{r}$$

where $R$ is a $3 \times 3$ matrix. Written out:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R \begin{pmatrix} x \\ y \\ z \end{pmatrix} \equiv \begin{pmatrix} R_{xx} & R_{xy} & R_{xz} \\ R_{yx} & R_{yy} & R_{yz} \\ R_{zx} & R_{zy} & R_{zz} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

In index notation:

$$x_i \to x_i' = R_{ij}\,x_j$$

Here we use the Einstein summation convention: sum over repeated indices.

Then since $r^2$ is invariant under rotations we have $(r')^2 = r^2 = \boldsymbol{r}^{\mathrm{T}}\boldsymbol{r}$.

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

Thus, the rotation matrices must satisfy $R^{\mathrm{T}}R = \mathbb{1}$. This we also write $R \in \mathrm{O}(3)$: O(3) is the group of $3 \times 3$ real matricees satisfying $R^{\mathrm{T}}R = \mathbb{1}$. In indices the requirement is $(R^{\mathrm{T}})_{ij}\,R_{jk} = \delta_{ik}$ or

$$R_{ji}\,R_{jk} = \delta_{ik}.$$

Then for $i = 1, k = 1$, say, we have $\sum_j\,(R_{j1})^2 = 1$. Squares sum to one: $R_{ij} \sim$ angles.

The invariance of $r^2$ can be reexpressed as the tensor invariance of $\delta_{ij}$ (the metric for the scalar product).

$$\delta_{ij} \quad \xrightarrow{R} \quad R_{ik}\,R_{jl}\,\delta_{kl} = (R\,\mathbb{1}\,R^{\mathrm{T}})_{ij}$$

Invariance of $\delta_{ij} \Rightarrow R\,\mathbb{1}R^{\mathrm{T}} = \mathbb{1} \Rightarrow R\,R^{\mathrm{T}} = \mathbb{1}$.

*Now:* Let us introduce covariant and contravariant vector (or indices):

$x^i$: contravariant vector
$x_i$: covariant vector

Then define (in vector space)

$$x'^{\,i} = x^j R_j{}^i$$

and then (in dual vector space)

$$x_i' = (R^{-1})_i{}^j x_j$$

since $x^i x_i$ is trivially invariant.

Check: $x'^i x'_i = x^j R_j{}^i (R^{-1})_i{}^k x_k = x^i x_i$.

*The point:* $x^i x_i$ then is invariant for any $3\times 3$ real $R$-matrix: $R \in \mathrm{GL}(3)$ with $\det(R) \neq 0$.

$\mathrm{GL}(n)$: $\det(R) \neq 0$.

$\mathrm{O}(n)$; $R\,R^{\mathrm{T}} = \mathbb{1} \Rightarrow (\det R)^2 = 1 \Rightarrow \det R = \pm 1$. If we choose $\det R = +1$ we get $\mathrm{SO}(n)$.

EXAMPLE from Quantum Mechanics.

Spin in Quantum Mechanics is represented by two-component complex "vectors":

$$\chi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad \alpha \in \mathbb{C}, \quad \beta \in \mathbb{C}.$$

The scalar products are

$$\chi^\dagger \chi = \begin{pmatrix} \bar{\alpha} & \bar{\beta} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = |\alpha|^2 + |\beta|^2.$$

Invariance is in terms of $2\times 2$ complex matrices $U$:

$$\chi \rightarrow \chi' = U\chi, \quad \chi^\dagger \rightarrow (\chi')^\dagger = \chi^\dagger U^\dagger$$

and $\chi^\dagger \chi$ is invariant:

$$(\chi')^\dagger \chi' = \chi^\dagger U^\dagger U \chi = \chi^\dagger \chi$$

$$\Rightarrow U^\dagger U = \mathbb{1}$$

i.e. $U \in \mathrm{U}(2)$, the group of $2\times 2$ unitary matrices.

Taking the determinant:

$$(\det U^\dagger)(\det U) = 1$$

Now the determinates are different, because of the complex conjugation.

$$\mathrm{e}^{-\mathrm{i}\alpha} \underbrace{\mathrm{e}^{\mathrm{i}\alpha}}_{\det U} = 1$$

$\Rightarrow \mathrm{U}(2) = \mathrm{U}(1) \times \mathrm{SU}(2)$ where $\mathrm{SU}(2)$ are the $2\times 2$ unit matrices with $\det U = +1$. $\mathrm{U}(1)$ is $\{\mathrm{e}^{\mathrm{i}\alpha}\}$.

*Note:* $U \in \mathrm{SU}(2)$:

$$U = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \Rightarrow |a|^2 + |b|^2 = 1 \Rightarrow U^\dagger U = \mathbb{1}$$

But this means that $\mathrm{SU}(2) \approx S^3$, the three-dimensional sphere:

$$a_1^2 + a_2^2 + b_1^2 + b_2^2 = 1$$

where $a = a_1 + \mathrm{i}\, a_2, b = b_2 + \mathrm{i}\, b_2$. Each group element in SU(2) corresponds to a point on the three-dimensional sphere $S^3$.

If SU(2) is isomorphic to $S^3$, what manifold is SO(3)?

*Answer:* $\mathrm{SO}(3) = \mathrm{RP}^3$: sort of one half of $S^3$, identifying points on the boundary (figure 4).


**Figure 4.** $\mathrm{RP}^3$ seen as one half of $S^3$, identifying points on the boundary.

*Note:* $S^3$ has *no* non-trivial loops. $\mathrm{RP}^3$ has $\mathbb{Z}_2$-non-trivial loops. (Some loops must be covered twice before being trivial.) That's an exercise.

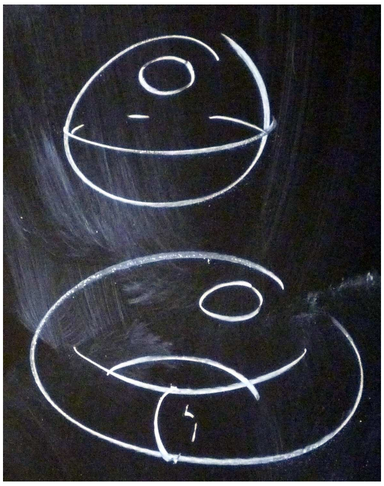

**Figure 5.** On the sphere $S^2$ all loops can be continuously contracted to a point (without leaving the surface). On the torus there are loops that can be continuously contracted to a point, but also non-trivial loops winding around the torus.

Back to $x^i$ and $x_i$. In General Relativity we have $x^\mu$ and $x_\mu$.

While $x^i x_i$ is invariant for any $R = \mathrm{GL}(3)$, I can do something similar that is even more general.

$$\mathrm{d} = \mathrm{d}x^\mu \, \partial_\mu$$

is invariant under *any* non-linear coordinate transformation (non-degenerate). It is called the exterior derivative. Using this Maxwell's equations can be written $F = \mathrm{d}A, \mathrm{d}F = 0, \mathrm{d} \star F = 0$.

Next time we will continue this discussion of real matrices forming groups, and complex matrices, and quaternionic matrices. (Octonions will be discussed later on.)