Double groups

David Kult and Patrik Thunström

June 8, 2007

Introduction

Let us begin by investigating how coordinate transformations in $\mathbb{R}^3$ affects different types of fields. A general coordinate transformation T act on a position vector $\mathbf{r} \in \mathbb{R}^3$ as $\mathbf{r}' = \{\mathbf{R}(T)|\mathbf{t}(T)\}\mathbf{r} = \mathbf{R}(T)\mathbf{r} + \mathbf{t}(T)$, where $\mathbf{R}(T)$ is a proper- or improper rotation and $\mathbf{t}(T)$ is a translation. Under such a coordinate transformation a scalar field $\psi(\mathbf{r})$ transforms as $\psi'(\mathbf{r}') = \psi(\mathbf{r}) = \psi(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}')$, whereas a vector field $\mathbf{A}(\mathbf{r})$ transform as

$$\mathbf{A}'(\mathbf{r}') = \mathbf{R}(T)\mathbf{A}(\mathbf{r}) = \mathbf{R}(T)\mathbf{A}(\{\mathbf{R}(T)|\mathbf{t}(T)\}^{-1}\mathbf{r}'). \tag{1}$$

The generalizations of this type of transformations to any-order tensor fields are straight forward, and include a 3^{n-1} dimensional representation of $O(3)$ for an order n tensor field.

In quantum mechanics, however, there exist a quantity that lie somewhere in between a scalar field and a vector field, namely the spinor. A spinor can be described as a two component quantity, where each component is a scalar field (i.e. a wave-function). A spinor $\boldsymbol{\psi}(\mathbf{r})$ is often represented by a column vector as

$$\boldsymbol{\psi}(\mathbf{r}) = \begin{pmatrix} \psi_1(\mathbf{r}) \\ \psi_2(\mathbf{r}) \end{pmatrix}. \tag{2}$$

An example of when spinors are necessary in quantum mechanics is when one wants to describe spin-1/2 particles. The internal degrees of freedom corresponding to the spin spans a two-dimensional Hilbert space, and the spatial degrees of freedom span the ordinary L^2 space. This results in a total Hilbert space where each point corresponds to a spinor (one can view the space of spinors as a tensor product between L^2 and a two-dimensional Hilbert space).

We now ask how spinors transform under a coordinate transformation in $\mathbb{R}^3$. Since there doesn't exist any faithful 2-dimensional representations of $O(3)$ we must look somewhere else. It turns out that somewhere else is $SU(2)$.

Map between SU(2) and SO(3)

Let us consider a 2-dimensional complex Hilbert space, $\mathcal{H}$, with a basis $\{|0\rangle, |1\rangle\}$. The Hilbert space is the state space of a spin 1/2 particle, and the vectors $|0\rangle$ and $|1\rangle$ corresponds to spin up and spin down in some predetermined direction. Any normalized vector in this space can be written as $|\psi\rangle = e^{i\gamma}\left(\cos(\theta/2)|0\rangle + e^{i\varphi}\sin(\theta/2)|1\rangle\right)$, where $\theta \in [0, \pi]$, and $\gamma, \varphi \in [0, 2\pi]$. However, since this Hilbert space corresponds to a quantum mechanical state space, it is a well known fact that the global phase factor $e^{i\gamma}$ is physically irrelevant, as it cannot influence any measurements. Therefore, a more appropriate space to consider is a 2-dimensional projective Hilbert space, $\mathcal{PH}$, defined by using the equivalence relation $|\psi\rangle \sim e^{i\phi}|\psi\rangle$, $\forall\phi \in \mathbb{R}$, such that $\mathcal{PH} = \mathcal{H}/\sim$. There exists a one-to-one map, Π, between projective Hilbert space and the space of rank 1 projectors $\mathcal{G}(2;1)$, given by

$$\begin{array}{rcl} \Pi : \mathcal{PH} & \rightarrow & \mathcal{G}(2;1) \\ [|\psi\rangle] & \mapsto & |\psi\rangle\langle\psi|. \end{array} \tag{3}$$

A way to visualize the spaces $\mathcal{G}(2;1)$ and $\mathcal{PH}$ is given by the so called Bloch vector representation. Each projector $|\psi\rangle\langle\psi|$ can be represented in the $\{|0\rangle, |1\rangle\}$ basis as the 2×2 matrix

$$\frac{1}{2}\begin{pmatrix} 1+\cos(\theta) & \sin(\theta)e^{-i\varphi} \\ \sin(\theta)e^{i\varphi} & 1-\cos(\theta) \end{pmatrix} = \frac{1}{2}\left(\mathbf{1} + \boldsymbol{n}\cdot\boldsymbol{\sigma}\right), \tag{4}$$

where $\boldsymbol{n} = (\cos(\varphi)\sin(\theta), \sin(\varphi)\sin(\theta), \cos(\theta))$ is called the Block vector, and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ where $\sigma_1, \sigma_2, \sigma_3$ are the usual Pauli matrices. Apparently, each projector can be viewed as a point $\boldsymbol{n}$ on the 3-dimensional sphere, and the direction of $\mathbf{n}$ corresponds to the direction of the spin in $\mathbb{R}^3$.

$SU(2)$ is the set of all unitary operators, u, acting on a 2-dimensional Hilbert space, such that $\det(u) = 1$. For each $u \in SU(2)$ we can construct a corresponding super operator $\mathcal{E}_u \in \mathcal{SL}(\mathcal{G}(2;1))$ acting on $\mathcal{G}(2;1)$ such that

$$\begin{array}{rcl} \mathcal{E}_u : \mathcal{G}(2;1) & \rightarrow & \mathcal{G}(2;1) \\ |\psi\rangle\langle\psi| & \mapsto & u|\psi\rangle\langle\psi|u^\dagger. \end{array} \tag{5}$$

It can be shown that $\mathcal{E}_u$ acting on $|\psi\rangle\langle\psi|$ results in a proper rotation of the Bloch vector. $\mathcal{E}_u$ therefore corresponds to a unique element T in $SO(3)$. This correspondence gives a mapping from $SU(2)$ to $SO(3)$ via $\mathcal{SL}(\mathcal{G}(2;1))$,

$$\begin{array}{rccccc} \Psi : & SU(2) & \rightarrow & \mathcal{SL}(\mathcal{G}(2;1)) & \rightarrow & SO(3) \\ & u & \mapsto & \mathcal{E}_u & \mapsto & T \end{array} \tag{6}$$

Note, however, that from the definition in eqn. (5) we have that $\mathcal{E}_u = \mathcal{E}_{-u}$, so the mapping from $SU(2)$ to $\mathcal{SL}(\mathcal{G}(2;1))$ is not one-to-one, but two-to-one. This makes the mapping Ψ two-to-one as well, taking both u and $-u$ to T.

Spinor transformations and double groups

Equipped with the mapping Ψ or, more precisely, with the inverse Ψ^{-1}, we are now ready to look at how spinors behave under coordinate transformations. Under a proper transformation $\{\mathbf{R}(T|\mathbf{t}(T))\}$ a spinor $\boldsymbol{\psi}(\mathbf{r})$ transforms as

$$\boldsymbol{\psi}'(\mathbf{r}') = \pm\mathbf{u}(\mathbf{R}(T))\boldsymbol{\psi}(\{\mathbf{R}(T)|\mathbf{t}(T))\}^{-1}\mathbf{r}'), \tag{7}$$

where $\pm\mathbf{u}(\mathbf{R}(T)) = \Psi^{-1}(\mathbf{R}(T))$ and the $\pm$-sign should not be interpreted as dual-valuedness, but rather as a freedom of choice regarding the sign.

This $\pm$-ambiguity is a result of the fact that Ψ^{-1} is a one-to-two mapping. On a formal level $\Psi^{-1}(\mathbf{R}(T)) = \{\tilde{\mathbf{u}}(\mathbf{R}(T)), \tilde{\tilde{\mathbf{u}}}(\mathbf{R}(T))\}$, where $\tilde{\mathbf{u}}(\mathbf{R}(T)) = -\tilde{\tilde{\mathbf{u}}}(\mathbf{R}(T))$. We are now free to define $\mathbf{u}(\mathbf{R}(T))$ as either $\tilde{\mathbf{u}}(\mathbf{R}(T))$ or $\tilde{\tilde{\mathbf{u}}}(\mathbf{R}(T))$, and taking the other choice as $-\mathbf{u}(\mathbf{R}(T))$. If we assume that this choice has been made for all transformations the operators $\mathbf{u}(\mathbf{R}(T)$ has the property

$$\mathbf{u}(\mathbf{R}_1(T))\mathbf{u}(\mathbf{R}_2(T)) \quad = \quad \pm\mathbf{u}(\mathbf{R}_1(T)\mathbf{R}_2(T)) \tag{8}$$

where the sign is decided from the sign convention.

The transformation law in eqn. (7) can be generalized to arbitrary coordinate transformations by defining for every rotation $\mathbf{R}(T)$ what is called the "proper part", $\mathbf{R}_p(T)$

$$\mathbf{R}_p(T) = \begin{cases} \mathbf{R}(T), & \text{if} \quad \mathbf{R}(T) \text{ is a proper rotation,} \\ -\mathbf{R}(T), & \text{if} \quad \mathbf{R}(T) \text{ is an improper rotation.} \end{cases} \tag{9}$$

The generalization reads

$$\boldsymbol{\psi}'(\mathbf{r}') = \pm\mathbf{u}(\mathbf{R}_p(T))\boldsymbol{\psi}(\{\mathbf{R}(T)|\mathbf{t}(T))\}^{-1}\mathbf{r}'). \tag{10}$$

In order to avoid having to use, $\pm$, all the time we may divide the transformation into two parts, defining the "spinor transformation operators" $\mathbf{O}(T)$ and $\mathbf{O}(\bar{T})$ as

$$\begin{cases} \boldsymbol{\psi}'(\mathbf{r}') = \mathbf{O}(T)\boldsymbol{\psi}(\mathbf{r}) = \mathbf{u}(\mathbf{R}_p(T))\boldsymbol{\psi}(\{\mathbf{R}(T)|\mathbf{t}(T))\}^{-1}\mathbf{r}'), \\ \boldsymbol{\psi}'(\mathbf{r}') = \mathbf{O}(\bar{T})\boldsymbol{\psi}(\mathbf{r}) = -\mathbf{u}(\mathbf{R}_p(T))\boldsymbol{\psi}(\{\mathbf{R}(T)|\mathbf{t}(T))\}^{-1}\mathbf{r}'). \end{cases} \tag{11}$$

Let us now show that if the set of coordinate transformations T form a group $\mathcal{G}$, then so does the set of operators $\mathbf{O}(T)$ and $\mathbf{O}(\bar{T})$. This can be shown by checking that the four group axioms are satisfied. We begin by noting that for any transformations T_1 and T_2

$$\begin{aligned} &\mathbf{O}(T_1)\mathbf{O}(T_2) = \mathbf{O}(\bar{T}_1)\mathbf{O}(\bar{T}_2) \\ &= \begin{cases} \mathbf{O}(T_1T_2), & \text{if} \quad \mathbf{u}(\mathbf{R}_p(T_1))\mathbf{u}(\mathbf{R}_p(T_2)) = +\mathbf{u}(\mathbf{R}_p(T_1T_2)) \\ \mathbf{O}(\overline{T_1T_2}), & \text{if} \quad \mathbf{u}(\mathbf{R}_p(T_1))\mathbf{u}(\mathbf{R}_p(T_2)) = -\mathbf{u}(\mathbf{R}_p(T_1T_2)), \end{cases} \end{aligned} \tag{12}$$

and

$$\begin{aligned} &\mathbf{O}(\bar{T}_1)\mathbf{O}(T_2) = \mathbf{O}(T_1)\mathbf{O}(\bar{T}_2) \\ &= \begin{cases} \mathbf{O}(T_1T_2), & \text{if} \quad \mathbf{u}(\mathbf{R}_p(T_1))\mathbf{u}(\mathbf{R}_p(T_2)) = -\mathbf{u}(\mathbf{R}_p(T_1T_2)) \\ \mathbf{O}(\overline{T_1T_2}), & \text{if} \quad \mathbf{u}(\mathbf{R}_p(T_1))\mathbf{u}(\mathbf{R}_p(T_2)) = +\mathbf{u}(\mathbf{R}_p(T_1T_2)), \end{cases} \end{aligned} \tag{13}$$

which follows from eqn. (8). Hence, the first axiom is satisfied. The second axiom, associativity, follows directly from the fact that $\mathbf{O}(T)$ are operators. The third axiom, i.e. that there exists an identity element, is fulfilled by the operator $\mathbf{O}(E)$, where E is the identity element in $\mathcal{G}$, and $\mathbf{u}(\mathbf{R}_p(E)) = \mathbf{1}$. Finally, $\mathbf{O}(T)^{-1}$ is either $\mathbf{O}(T')$ or $\mathbf{O}(\bar{T}')$, where $T' = T^{-1}$, depending on the sign conventions. The same is true for $\mathbf{O}(\bar{T})^{-1}$, and therefore the fourth axiom is also fulfilled.

As can be seen in eqn. (11) the two operators $\mathbf{O}(T)$ and $\mathbf{O}(\bar{T})$ only differ in their dependence on the rotational part of T. It is therefore convenient to introduce the notation $\mathbf{O}(T) = \mathbf{O}([\mathbf{R}(T)|\mathbf{t}(T)])$, $\mathbf{O}(\bar{T}) = \mathbf{O}([\bar{\mathbf{R}}(T)|\mathbf{t}(T)])$, where $[\mathbf{R}(T)|\mathbf{t}(T)]$ and $[\bar{\mathbf{R}}(T)|\mathbf{t}(T)]$ can be seen as "generalized" coordinate transformations corresponding to $\{\mathbf{R}(T)|\mathbf{t}(T)\}$. The set of generalized coordinate transformations is isomorphic to the set of operators $\mathbf{O}(T)$ and $\mathbf{O}(\bar{T})$, and one can show that it also constitutes a group by defining the product of two generalized coordinate transformations in the same spirit as eqns. (12) and (13) as

$$
\begin{aligned}
&[\mathbf{R}(T_1)|\mathbf{t}(T_1)]\,[\mathbf{R}(T_2)|\mathbf{t}(T_2)] = \left[\bar{\mathbf{R}}(T_1)|\mathbf{t}(T_1)\right]\,\left[\bar{\mathbf{R}}(T_2)|\mathbf{t}(T_2)\right] \\
&= \begin{cases} [\mathbf{R}(T_1T_2)|\mathbf{t}(T_1T_2)]\,, & \text{if} \quad \mathbf{u}(\mathbf{R}_p(T_1))\mathbf{u}(\mathbf{R}_p(T_2)) = +\mathbf{u}(\mathbf{R}_p(T_1T_2)) \\ \left[\bar{\mathbf{R}}(T_1T_2)|\mathbf{t}(T_1T_2)\right]\,, & \text{if} \quad \mathbf{u}(\mathbf{R}_p(T_1))\mathbf{u}(\mathbf{R}_p(T_2)) = -\mathbf{u}(\mathbf{R}_p(T_1T_2)), \end{cases}
\end{aligned}
$$

and

$$
\begin{aligned}
&\left[\bar{\mathbf{R}}(T_1)|\mathbf{t}(T_1)\right]\,[\mathbf{R}(T_2)|\mathbf{t}(T_2)] = [\mathbf{R}(T_1)|\mathbf{t}(T_1)]\,\left[\bar{\mathbf{R}}(T_2)|\mathbf{t}(T_2)\right] \\
&= \begin{cases} [\mathbf{R}(T_1T_2)|\mathbf{t}(T_1T_2)]\,, & \text{if} \quad \mathbf{u}(\mathbf{R}_p(T_1))\mathbf{u}(\mathbf{R}_p(T_2)) = -\mathbf{u}(\mathbf{R}_p(T_1T_2)) \\ \left[\bar{\mathbf{R}}(T_1T_2)|\mathbf{t}(T_1T_2)\right]\,, & \text{if} \quad \mathbf{u}(\mathbf{R}_p(T_1))\mathbf{u}(\mathbf{R}_p(T_2)) = +\mathbf{u}(\mathbf{R}_p(T_1T_2)). \end{cases}
\end{aligned}
$$

This group, let us call it $\mathcal{G}^D$, is known as the double group corresponding to $\mathcal{G}$.

IR's of double groups

From the multiplication law of the double group $\mathcal{G}^D$ we have that $[\bar{E}|0]$ must commute with every element. Hence, for any IR Γ we must have $\Gamma([\bar{E}|0]) = c\mathbf{1}$, where c is a constant. Furthermore, we have that $[\bar{E}|0][\bar{E}|0] = [E|0]$, which entails $c^2 = 1$, or in other words $c = \pm 1$. If $c = 1$ we get from the multiplication laws that $\Gamma([\mathbf{R}(T)|\mathbf{t}(T)]) = \Gamma([\bar{\mathbf{R}}(T)|\mathbf{t}(T)])$. This allows us to use the IR's of $\mathcal{G}$ to construct IR's of $\mathcal{G}^D$. If Γ' is a IR of $\mathcal{G}$ we simply define $\Gamma'(\{\mathbf{R}(T)|\mathbf{t}(T)\}) = \Gamma([\mathbf{R}(T)|\mathbf{t}(T)]) = \Gamma([\bar{\mathbf{R}}(T)|\mathbf{t}(T)])$. If $c = -1$, on the other hand, we get that $\Gamma([\mathbf{R}(T)|\mathbf{t}(T)]) = -\Gamma([\bar{\mathbf{R}}(T)|\mathbf{t}(T)])$. In this case we can not directly relate the IR's of $\mathcal{G}^D$ with IR's of $\mathcal{G}$. If we tried for example to define $\Gamma([\mathbf{R}(T)|\mathbf{t}(T)]) = \Gamma'(\{\mathbf{R}(T)|\mathbf{t}(T)\})$, we could get

$$
\begin{aligned}
&\Gamma([\mathbf{R}(T_1T_2)|\mathbf{t}(T_1T_2)]) = \Gamma'(\{\mathbf{R}(T_1T_2)|\mathbf{t}(T_1T_2)\}) = \\
&\Gamma'(\{\mathbf{R}(T_1)|\mathbf{t}(T_1)\})\Gamma'(\{\mathbf{R}(T_2)|\mathbf{t}(T_2)\}) = \\
&\Gamma([\mathbf{R}(T_1)|\mathbf{t}(T_1)])\Gamma([\mathbf{R}(T_2)|\mathbf{t}(T_2)]) = \\
&\Gamma([\mathbf{R}(T_1)|\mathbf{t}(T_1)][\mathbf{R}(T_2)|\mathbf{t}(T_2)]) = \\
&\Gamma([\bar{\mathbf{R}}(T_1T_2)|\mathbf{t}(T_1T_2)]) = -\Gamma([\mathbf{R}(T_1T_2)|\mathbf{t}(T_1T_2)]).
\end{aligned} \tag{14}
$$

The IR's of $\mathcal{G}^D$ which are not directly related to IR's of $\mathcal{G}$ are called extra representations. These are often the ones that are most interesting since it can be shown that if a set of spinors is a basis for a representation, then the representation must be an extra representation.

The double crystallographic point groups where thoroughly investigated by Opechowski in 1940. He derived the two following general rules regarding the classes of double point groups:

(i) If a set of proper or improper rotations $\{\mathbf{R}(T)|\mathbf{0}\}$ through $2\pi/n$ form a class in the single group, then the set of rotations $[\mathbf{R}(T)|\mathbf{0}]$ and $[\bar{\mathbf{R}}(T)|\mathbf{0}]$ form two separate classes in the double group.

(ii) There is one exception of (i), namely that if $n = 2$, then $[\mathbf{R}(T)|\mathbf{0}]$ and $[\bar{\mathbf{R}}(T)|\mathbf{0}]$ lie in the same class if and only if there exists in the single group a proper or improper rotation through π around an axis perpendicular to the axis of $\{\mathbf{R}(T)|\mathbf{0}\}$.

We end this section with an example of a character table for the double point group D_4^D. Its classes are [1]:

$$\begin{array}{ll}
\mathcal{C}_1 = \{[\mathbf{E}|\mathbf{0}]\} & \mathcal{C}_2 = \{[\bar{\mathbf{E}}|\mathbf{0}]\} \\
\multicolumn{2}{l}{\mathcal{C}_3 = \{[\mathbf{C}_{2x}|\mathbf{0}], [\mathbf{C}_{2z}|\mathbf{0}], [\bar{\mathbf{C}}_{2x}|\mathbf{0}], [\bar{\mathbf{C}}_{2z}|\mathbf{0}]\}} \\
\mathcal{C}_4 = \{[\mathbf{C}_{2y}|\mathbf{0}], [\bar{\mathbf{C}}_{2y}|\mathbf{0}]\} & \mathcal{C}_5 = \left\{[\mathbf{C}_{4y}|\mathbf{0}], \left[\mathbf{C}_{4y}^{-1}|\mathbf{0}\right]\right\} \\
\mathcal{C}_6 = \left\{[\bar{\mathbf{C}}_{4y}|\mathbf{0}], \left[\bar{\mathbf{C}}_{4y}^{-1}|\mathbf{0}\right]\right\} & \mathcal{C}_7 = \{[\mathbf{C}_{2c}|\mathbf{0}], [\mathbf{C}_{2d}|\mathbf{0}], [\bar{\mathbf{C}}_{2c}|\mathbf{0}], [\bar{\mathbf{C}}_{2d}|\mathbf{0}]\}
\end{array}$$

and the character table is [1]:

	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$	$\mathcal{C}_7$
$\mathbf{\Gamma}^1$	1	1	1	1	1	1	1
$\mathbf{\Gamma}^2$	1	1	1	1	-1	-1	-1
$\mathbf{\Gamma}^3$	1	1	-1	1	1	1	-1
$\mathbf{\Gamma}^4$	1	1	-1	1	-1	-1	1
$\mathbf{\Gamma}^5$	2	2	0	-2	0	0	0
$\mathbf{\Gamma}^6$	2	-2	0	0	$\sqrt{2}$	$-\sqrt{2}$	0
$\mathbf{\Gamma}^7$	2	-2	0	0	$-\sqrt{2}$	$\sqrt{2}$	0

Note that the IR's Γ^6 and Γ^7 are the extra representations, and that the character for classes containing both $[\mathbf{R}(T)|\mathbf{0}]$ and $[\bar{\mathbf{R}}(T)|\mathbf{0}]$ (i.e. class 3,4, and 7) is 0 as it must be since $\chi^{6,7}([\mathbf{R}(T)|\mathbf{0}]) = -\chi^{6,7}([\bar{\mathbf{R}}(T)|\mathbf{0}])$

Bibliography

[1] J.F Cornwell, *Group Theory in Physics* Vol. I (Academic Press, Bury St Edmunds, Suffolk) 1984.