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Lecture notes for FYS610 Many particle Quantum Mechanics

Note 13, 22.3 2017

Additions and comments to *Quantum Field Theory and the Standard Model* by Matthew D. Schwartz (2014)

Representations of the rotation group

To illustrate the results of lecture note 12, we shall work out the commutator algebra for the rotation group, SO(3), bu considering the *defining representation*, as 3×3 real orthogonal matrices $R(\boldsymbol{\phi})$, which is a particular case of a unitary transformation. In order to calculate S^i, eq. (12.15) shows that it suffices to consider rotations about the coordinate axes:

$$R(\phi_1 \mathbf{e}_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi_1 & -\sin\phi_1 \\ 0 & \sin\phi_1 & \cos\phi_1 \end{pmatrix}, \qquad R(\phi_2 \mathbf{e}_2) = \begin{pmatrix} \cos\phi_2 & 0 & \sin\phi_2 \\ 0 & 1 & 0 \\ -\sin\phi_2 & 0 & \cos\phi_2 \end{pmatrix},$$
$$R(\phi_3 \mathbf{e}_3) = \begin{pmatrix} \cos\phi_3 & -\sin\phi_3 & 0 \\ \sin\phi_3 & \cos\phi_3 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{13.1}$$

The generators then follow from $T^i = -\mathrm{i}(\partial R(\phi \mathbf{e}_i)/\partial \phi_i)_{\boldsymbol{\phi}=0}$:

$$T^1 = -\mathrm{i}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad T^2 = -\mathrm{i}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad T^3 = -\mathrm{i}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{13.2a}$$

We note that we have $\mathbf{T}^2 = {T^1}^2 + {T^3}^2 + {T^2}^2 = 2\mathbb{1}_3$. This quantity is thus an invariant under rotation, since it commutes with all rotation matrices. Eq. (13.2) can be written more compactly as:

$$T^i_{jk} = \mathrm{i}\epsilon_{ijk}\,. \tag{13.2b}$$

This makes it very easy to check the commutation relations, using $\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$ and the antisymmetry of ϵ_{ijk} under permutations of the indices:

$$\begin{aligned} \left([T^i, T^j]\right)_{kl} &= -\epsilon_{ikm}\epsilon_{jml} - \epsilon_{jkm}\epsilon_{iml} = \delta_{il}\delta_{kj} - \delta_{ij}\delta_{kl} - \delta_{jl}\delta_{ki} + \delta_{ji}\delta_{kl} \\ &= \delta_{il}\delta_{jk} - \delta_{jl}\delta_{ik} = -\epsilon_{mij}\epsilon_{mkl} = \mathrm{i}\epsilon_{mij}T^m_{kl}\,, \end{aligned} \tag{13.3}$$

showing that the structure constants of the group are indeed $c_{ijk} = \epsilon_{ijk}$, as stated in eq. (12.16).

An important observation is that since the set of rotations around a fixed axis constitute an Abelian group, we can actually immediately find a formula for *finite rotations* around a fixed axis. In that case we can immediately copy the analysis we did in lecture notes 12, and find:

$$R(\phi_3 \mathbf{e}_3) = e^{\mathrm{i}\phi_3 T^3} = \sum_{n=0}^{\infty} \frac{(\mathrm{i}\phi_3)^n}{n!} T^{3\,n} \,.$$

But for $n > 0$ we find:

$$T^{3\,2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = T^{3\,2n}, \quad T^{3\,2n+1} = T^3 \,,$$

so we can evaluate the sum in eq.(13.4):

$$\begin{aligned} R(\phi_3 \mathbf{e}_3) &= \mathbb{1}_3 + iT^3 \sum_{n=0}^{\infty} (-1)^n \frac{(\phi_3)^{2n+1}}{(2n+1)!} + T^{3\,2} \sum_{n=1}^{\infty} (-1)^n \frac{(\phi_3)^{2n}}{(2n)!} \\ &= \mathbb{1}_3 + iT^3 \sin\phi_3 + T^{3\,2}(\cos\phi_3 - 1) = \begin{pmatrix} \cos\phi_3 & -\sin\phi_3 & 0 \\ \sin\phi_3 & \cos\phi_3 & 0 \\ 0 & 0 & 1 \end{pmatrix} . \end{aligned} \tag{13.1$'$}$$

which is the correct result. But there is nothing special with the z-axis, and we might habe performed the same manipulation for an arbitrary linear combination $\boldsymbol{\phi}\cdot\mathbf{T}$, obtaining the formula for a finite rotation around any axis. Thus, knowing the generators, we can, at least in principle, calculate the result of any finite transformation (cf. *Goldstein* sec. 4.7). Furthermore, this means that we can write any rotation matrix as:

$$R(\boldsymbol{\phi}) = e^{\mathrm{i}\boldsymbol{\phi}\cdot\mathbf{T}} \,, \tag{13.4}$$

where $\mathbf{T} = [T^2, T^2, T^3]$.

To apply the above formulas in quantum mechanics, it is very useful to have a representation where one of the generators, customarily one chooses T^3, to be diagonal, since they represent physical observables. No transformation involving only real matrices can bring T^3 on a diagonal form. But this is easily done by a unitary transformation. The eigenvalue equation for T_3 is simply:

$$\text{Det }(T^3 - \lambda\mathbb{1}_3) = -\lambda^3 + \lambda = 0 \qquad \lambda = -1, 0, 1 \,. \tag{13.5}$$

The eigenvectors are easily found, and so T^3 can be diagonalized. We shall follow tradition, calling the quantum mechanical generators of the rotation group for S^i, and reserving J^i for the full Euclidean group, including the translations:

$$\begin{aligned} &S^3 = V^\dagger T^3 V = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ -\mathrm{i} & 0 & \mathrm{i} \\ 0 & \sqrt{2} & 0 \end{pmatrix} , \\ &S^1 = V^\dagger T^1 V = \frac{\mathrm{i}}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} , \qquad S^2 = V^\dagger T^2 V = \frac{\mathrm{i}}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} . \end{aligned} \tag{13.6}$$

We obviously still have $\mathbf{S}^2 = 2\mathbb{1}_2$.

The above shows the explicit construction of generators for the rotation group in its defining, or fundamental representation. But based on the fundamental commutation relations, one can find many other irreducible representations. Since $[\mathbf{S}^2, S^3] = 0$, one can construct a basis where these to operators are simultaneously diagonal. Since $\mathbf{S}^2$ commutes with all rotation operators, its value cannot be changed by a rotation, so σ can be used to label the irreducible representations. Thus we introduce a basis $\{|\,\sigma, m\,\rangle\}$ with the properties

$$\mathbf{S}^2|\,\sigma, m\,\rangle = \sigma|\,\sigma, m\,\rangle \qquad S^3|\,\sigma, m\,\rangle = m|\,\sigma, m\,\rangle\,. \tag{13.7}$$

Also, we note that if m is an eigenvalue of S^3, we must have $m^2 \le \sigma$ from the definition of $\mathbf{S}^2$. The trick is now to introduce the *ladder operators*, $S^{\pm} = S^1 \pm \mathrm{i}S^2$. These obviously commute with $\mathbf{S}^2$, but in addition it follows from the Lie algebra that:

$$[S^3, S^{\pm}] = \pm S^{\pm} \qquad \Longrightarrow \qquad S^3\left(S^{\pm}|\,\sigma, m\,\rangle\right) = (m \pm 1)\left(S^{\pm}|\,\sigma, m\,\rangle\right)\,. \tag{13.8}$$

Hence we must have $S^{\pm}|\,\sigma, m\,\rangle = c^{\pm}(\sigma, m)|\,\sigma, m \pm 1\,\rangle$ for some constants $c^{\pm}(\sigma, m)$. Furthermore, since

$$\begin{aligned} S^{\pm}S^{\mp}|\,\sigma, m\,\rangle &= \left({S^1}^2 + {S^2}^2 \mp \mathrm{i}[S^1, S^2]\right)|\,\sigma, m\,\rangle = \left(\mathbf{S}^2 - {S^3}^2 \pm S^3\right)|\,\sigma, m\,\rangle \\ &= (\sigma - m^2 \pm m)|\,\sigma, m\,\rangle\,. \end{aligned} \tag{13.9}$$

This tells us that when we go up and down the ladder, increasing and decreasing m, we will always come back to the same states. Thus, there is only one state for each m which is connected to other states by the generators. Now we have already noted that $m^2 \le \sigma$. This means that if σ is finite, there is a maximal m, which we shall call s. For $m = s$ we must then have $S^+|\,\sigma, s\,\rangle = 0$. From eq. (13.9) this leads to:

$$0 = S^-\left(S^+|\,\sigma, s\,\rangle\right) = (\sigma - s^2 - s)|\,\sigma, m\,\rangle \qquad \Longrightarrow \qquad \sigma = s(s+1)\,. \tag{13.10}$$

In an analogous manner we find that when σ is finite, there is some minimum $m = -s'$ such that $S^-|\,\sigma, -s'\,\rangle = 0$, implying $\sigma = (-s')(-s'-1) = s'(s'+1)$, so we must have $s' = s$. Furthermore, successive applications of S^+ takes us from $m = -s$ to $m = s$ in steps of 1, so $2s+1$ must be an integer, *i.e.* s must be integer or half integer. Thus, the Lie algebra of the rotation group has representations of any integer dimension, labeled by an integer or half integer s, and containing $2s+1$ states with $m = -s \dots s$. The defining three-dimensional representation corresponds to $s = 1$.

But we have not proven that all this representation of the algebra also gives rise to an acceptable representation of the group. To do this, we must find the generators of the representations explicitly. This is actually fairly straightforward. We shall later be particularly interested in the case $s = \frac{1}{2}$, so let us perform the construction in this case. We then have only two basis vectors for the irreducible representation, which can be taken to be:

$$|\,\tfrac{1}{2}, \tfrac{1}{2}\,\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\,, \qquad |\,\tfrac{1}{2}, -\tfrac{1}{2}\,\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\,. \tag{13.11}$$

Since S^3 should be diagonal, with eigenvalues $\pm\frac{1}{2}$, we have:

$$S^3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{13.12}$$

To find S^1 and S^2, we exploit that since $S^\pm$ are ladder operators, they can be written, up to constants, as:

$$\begin{gathered} S^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} , \qquad S^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} ; \\ S^+\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 , \quad S^+\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad S^-\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \quad S^-\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 . \end{gathered} \tag{13.13}$$

We find S^1 and S^2 as:

$$S^1 = \frac{1}{2}\left(S^+ + S^-\right) = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \qquad S^2 = \frac{1}{2\mathrm{i}}\left(S^+ - S^-\right) = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} . \tag{13.14}$$

These generators are mostly written in terms of the *Pauli matrices*, σ^i, as:

$$S^i = \frac{1}{2}\sigma^i . \tag{13.15}$$

We have even obtained them in their standard form. They satisfy $\mathrm{Trace}\sigma^i = 0$ and the simple algebra:

$$\sigma^i\sigma^j = \delta_{ij}\mathbb{1}_2 + \mathrm{i}\epsilon_{ijk}\sigma^k \quad \Longleftrightarrow \quad [\sigma^i, \sigma^j] = 2\mathrm{i}\epsilon_{ijk}\sigma^k, \quad \{\sigma^i, \sigma^j\} = 2\delta_{ij}\mathbb{1}_2 . \tag{13.16}$$

The commutator relation here of course just reflects the Lie algebra. We then find the group transformation matrices for the $s = \frac{1}{2}$ representation in the same manner as for the fundamental representation, eqs. (13.1'), using ${\sigma^i}^2 = \mathbb{1}_2$:

$$D^{\frac{1}{2}}(\phi\mathbf{e}_3) = e^{\frac{1}{2}\phi\sigma^3} = \mathbb{1}_2\cos\left(\frac{\phi}{2}\right) + \mathrm{i}\sigma^3\sin\left(\frac{\phi}{2}\right) = \begin{pmatrix} e^{\mathrm{i}\frac{1}{2}\phi} & 0 \\ 0 & e^{-\mathrm{i}\frac{1}{2}\phi} \end{pmatrix} . \tag{13.17a}$$

The corresponding result for an arbitrary rotation with $\boldsymbol{\phi} = \phi\mathbf{n}$ is then:

$$D^{\frac{1}{2}}((\phi)) = e^{\frac{1}{2}\phi\mathbf{n}\cdot\boldsymbol{\sigma}} = \mathbb{1}_2\cos\left(\frac{\phi}{2}\right) + \mathrm{i}\,\mathbf{n}\cdot\boldsymbol{\sigma}\sin\left(\frac{\phi}{2}\right) . \tag{13.17b}$$

In particular, from this result we see that for $\phi = 2\pi$, we have

$$D^{\frac{1}{2}}(2\pi\mathbf{n}) = -\mathbb{1}_2 \tag{13.18}$$

independently of the rotation axis, $\mathbf{n}$. Thus the $s = \frac{1}{2}$ representation is not a true representation of the rotation group, but only a projective representation. We have thus found that a representation of the Lie algebra is not necessarily a representation of the group it is derived from.

The above construction can be carried through for any s. One chooses $S^3 = \mathrm{Diag}(s, s - 1 \ldots - s)$, For S^+ one can pick a matrix with the only non-zero elements being one's in the positions one step above the main diagonal, times some constant, and then chose $S^- = S^\dagger$. From this S^1 and S^2 are calculated as in eq. (13.14), and the remaining constant chosen so the Lie algebra is fulfilled. Finally, the representation matrices are obtained like in eqs. (13.17), although the actual expressions become more cumbersome for $s > 1$. We will discover that for a full rotation, $\phi = 2\pi$ about any axis, we have:

$$D^s(2\pi\mathbf{n}) = (-1)^{2s}\mathbb{1}_{2s+1}\,. \tag{13.19}$$

Thus we only have a projective representation for half integer s. But for integer s all representations are true. Thus we recover the well known result that the finite dimensional irreducible unitary representation of the rotation groups ore of odd dimensions, while there are even-dimensional projective representations.

A wavefunction which can be written as:

$$|\,\psi\,\rangle = \sum_{m=-s}^{s} \psi_m^{\alpha;s}|\,\alpha; s\,\rangle|\,s, m\,\rangle \tag{13.20}$$

(no sum over s) in the notation of the lecture notes 12, is said to transform according to an irreducible representation of the group, only components with different m's are mixed by a rotation. Similarly, an operator with $2s+1$ components O_m^s, transforming as:

$$U(\boldsymbol{\phi})T_m^s U(\boldsymbol{\phi})^\dagger = \sum_{m'=-s}^{s} T_{m'}^s D_{m'm}^s(\boldsymbol{\phi})\,, \tag{13.21}$$

is said to transform under the s-representation.

Just like we did for translations, we can construct wavefunctions for the simplest possible quantum system with three-dimensional rotational invariance, a sphere fixed at some point since we have not considered translations. This will indeed be a model of a spinning sphere, and if we calculate the angular momentum operators, $\mathbf{J}$, from Noether's theorem, we will indeed find that $\mathbf{J} = \mathbf{S}$, so we can identify $\mathbf{S}$ with the intrinsic angular momentum, or *spin*. We call s and m the spin quantum numbers, and from the postulate that elementary particles must transform according to irreducible representations of the relevant symmetry groups, we conclude that elementary particles must transform according to some group representation labelled by s. We might add here that it mathematically there is nothing inconsistently with $\sigma = \infty$, *i.e.* representations of infinite spin with infinitely many values of m. But they are very hard to interpret physically, and no use of them has cropped up in physics so far.

We have to add some comments of other representations of the rotation group. In classical mechanics we hardly ever encounter the irreducible representations constructed above, except for the cases $s = 0$, scalars, and $s = 1$, which is the vector representation. For more complicated cases we use *tensors*. A tensor under the rotation group of rank m transforms under a rotation as:

$$T'_{i_1 \ldots i_n} = R_{i_1 j_1} \ldots R_{i_n j_n} T_{j_1 \ldots j_n}\,. \tag{13.22}$$

This is not a linear transformation at all for $n > 1$, or so rather unsuitable for quantum mechanical use, although it is perfectly find for operators. Furthermore, it does not even represent a single irreducible representation in the general case. This is easily seen for $n = 2$, in which case T_{ij} is simply a matrix. We know that a general matrix cam always be split in it symmetric and antisymmetric part:

$$T = T^S + T^A = \frac{1}{2}(T + T^{\mathsf{T}}) + \frac{1}{2}(T - T^{\mathsf{T}})\,. \tag{13.23}$$

where T^{T} is the transposed matrix. Since rotations do not mix the two parts, they transform under independent irreducible representations. Indeed the antisymmetric part is equivalent to a vector, which is easily constructed using the Levi-Civita tensor:

$$T_i = \epsilon_{ijk} T^A_{jk} = \epsilon_{ijk} T_{jk} \qquad \Leftrightarrow \qquad T^A_{ij} = \epsilon_{ijk} T_k\,. \tag{13.24}$$

where we have used that $\epsilon_{ijk} T^S_{jk} = 0$. Thus the antisymmetric part transforms as a vector ($s = 1$), and so is irreducible. But the symmetric part is still reducible, because its trace is invariant under rotations, and so transform as a scalar, $s = 0$, $T'_{ii} = T_{ii}$. The remaining part forms a traceless symmetric matrix,

$$T^T_{ij} = T^S_{ij} - \frac{1}{3}\delta_{ij} T_{kk}\,. \tag{13.25}$$

This has 5 independent components, and transforms under the $s = 2$ irreducible representation. This representation is therefore sometimes referred to as the tensor representation of the rotation group. One easily checks that the number of parameters is correct: A 3×3 matrix has 9 independent components, and $9 = 1 + 3 + 5$. We shall, however, not work out the detailed mapping from tensor components to the spin eigenstates.

A last very important issue which we will only mention is the transformation properties of composite states. If we have two states, say $|\, s_1, m_1 \,\rangle$ and $|\, s_2, m_2 \,\rangle$, how does the composite system $|\, s_1, m_1 \,\rangle |\, s_2, m_2 \,\rangle$ transform. Such combinations are very important, *i.e.* when we combine electronic wavefunctions in an atom or a solid, nucleons in a nucleus, or quarks in a nucleon. The answer is given by the *Clebsh–Gordan* series, which states that the direct product of the two states expands as:

$$|\, s_1, m_1 \,\rangle |\, s_2, m_2 \,\rangle = \sum_{j=|s_1-s_2|}^{s_1+s_2} \sum_{m=-j}^{j} \langle s_1 s_2 m_1 m_2 | s_1 s_2 j m \rangle |\, j, m \,\rangle\,. \tag{13.26}$$

The coefficients $\langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle$ are known as the *Clebsh–Gordan coefficients.* There is a vast literature about them, and their generalizations. The main point to remember is that the direct product of two representations give rise to states transforming according to *all irreducible representations between* $|s_1 - s_2|$ *and* $s_1 + s_2$. The corresponding result for the representation matrices themselves is:

$$D^{s_1}_{m'_1 m_1}(\boldsymbol{\phi}) D^{s_2}_{m'_2 m_2}(\boldsymbol{\phi}) = \sum_{j=|s_1-s_2|}^{s_1+s_2} \sum_{m,m'=-j}^{j} \langle s_1 s_2 m_1 m_2 | s_1 s_2 j m \rangle \langle s_1 s_2 m'_1 m'_2 | s_1 s_2 j m \rangle D^{j}_{m' m}(\boldsymbol{\phi})\,. \tag{13.27}$$