

Introduction to Symmetries

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Lecture 2:

Rotations and Angular Momentum.

We are going to follow very closely what we did for translations. To conform with most people's conventions we shall define our "positive rotation" as a rotation of the axes through a negative angle (i.e. clockwise). (In the case of translations, the analogous definition would be that whereas previously we said $x' = x - a$, now we will be saying $x' = x + a$, so the corresponding operator $\hat{U}_x(a)$ is $\hat{U}_x(a) = e^{-ia\hat{p}/\hbar}$.) Consider then such a rotation about the z-axis:

$$\begin{aligned}x' &= x \cos \alpha - y \sin \alpha \\y' &= x \sin \alpha + y \cos \alpha \\z' &= z\end{aligned}$$

i.e.

$$\mathbf{r}' = \mathbf{R}_z(\alpha) \mathbf{r}$$

where

$$\mathbf{R}_z(\alpha) = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \mathbf{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

Generally, $\mathbf{r}' = \mathbf{R}\mathbf{r}$ where \mathbf{R} is any real 3x3 matrix such that $\mathbf{r}'^T \mathbf{r}' = \mathbf{r}^T \mathbf{r}$: the length of the vector \mathbf{r} is unchanged under a rotation. We can rewrite this as

$$\mathbf{r}'^T \mathbf{r}' = (\mathbf{R}\mathbf{r})^T (\mathbf{R}\mathbf{r}) = \mathbf{r}^T \mathbf{R}^T \mathbf{R} \mathbf{r} = \mathbf{r}^T \mathbf{r}.$$

The last equality has to be true for *all* x, y, z varying independently of each other, and this can only be the case if $\mathbf{R}^T \mathbf{R} = \mathbf{I}$. All such 3 x 3 matrices represent *rotations*. Taking the determinant of both sides of this last equation, we get

$$\begin{aligned}\det(\mathbf{R}^T \mathbf{R}) &= \det(\mathbf{I}) = +1 \\ \Rightarrow \det(\mathbf{R}^T) \cdot \det(\mathbf{R}) &= +1.\end{aligned}$$

Note that it is a standard result that the determinant of a matrix equals the determinant of the transpose of the same matrix, so

$$(\det(\mathbf{R}))^2 = +1,$$

and then

$$\det(\mathbf{R}) = \pm 1.$$

Those \mathbf{R} 's with $\det(\mathbf{R}) = -1$ are effectively a combination of a parity transformation/reflection:

$$\begin{aligned}x &\rightarrow x' = -x \\y &\rightarrow y' = -y \\z &\rightarrow z' = -z\end{aligned}$$

followed by/preceded by a rotation (the reflection and rotation operations commute because the reflection operation is simply a -1 multiplicative factor). We only deal with continuous symmetries in this course so we forget about \mathbf{R} 's

with $\det(\mathbf{R}) = -1$. We shall stick to \mathbf{R} 's with $\det(\mathbf{R}) = +1$; these are referred to as “proper rotations,” or “special” - no reflections.

[Check that $\mathbf{R}_z^T(\alpha) \mathbf{R}_z(\alpha) = \mathbf{I}$ and $\det(\mathbf{R}_z(\alpha)) = +1$]

The set of all matrices \mathbf{R} such that $\mathbf{R}^T \mathbf{R} = \mathbf{I}$ and $\det(\mathbf{R}) = +1$ form a group called SO(3). “S” is for “special”, meaning $\det(\mathbf{R}) = +1$; “O” is for “orthogonal” meaning $\mathbf{R}^T \mathbf{R} = \mathbf{I}$; and “3” is for three real dimensions.

A number of rules (“group axioms”) have to be satisfied before any old set of things constitutes a group. One is that there should be a rule for associating two elements in the set (a “binary operation”) such that the so-associated pair is itself one of the elements in the set (“the set is closed under a binary operation”). In our case, the binary operation is matrix multiplication, and closure under this means that if we take a rotation matrix and multiply it by another rotation matrix (both members of SO(3)) then the resulting matrix is also a rotation and a member of SO(3).

A second group axiom is that every element should have an inverse which is in the group. This is easy to see for $\mathbf{R}_z(\alpha)$: if I rotate by α say the inverse matrix rotates by $-\alpha$ and both are clearly in SO(3). You can generalise this to more complicated SO(3) rotations, and the fact is that all such rotations have an inverse also in SO(3).

Groups must also by definition contain an identity. In our case this is obviously:

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The fourth and final axiom in the definition of a group is that the binary operation must be associative. In our case this means simply

$$\mathbf{R}_1 (\mathbf{R}_2 \mathbf{R}_3) = (\mathbf{R}_1 \mathbf{R}_2) \mathbf{R}_3 \quad .$$

Infinitesimal rotations are of particular interest in the study of rotation groups:

$$\mathbf{r} \rightarrow \mathbf{r}' = \mathbf{r} + \mathbf{a} \times \mathbf{r}$$

where $\mathbf{a} = \epsilon \mathbf{n}$, which is a rotation through the infinitesimal angle ϵ about an axis along the unit vector \mathbf{n} . For instance if $\mathbf{n} = (0, 0, 1)$ (a unit vector along the z-axis) then:

$$\begin{aligned} x' &= x - \epsilon y \\ y' &= y + \epsilon x \\ z' &= z \end{aligned}$$

which is the same as what we would get using $\mathbf{R}_z(\alpha)$ in the limit $\alpha \rightarrow \epsilon$ i.e. $\sin \epsilon \rightarrow \epsilon$ and $\cos \epsilon \rightarrow 1$.

So we can do coordinate transformations. How do they affect the Physics? The key question is: *What wavefunction will the people in the primed frame need to use, so as to describe consistently the same physics as people in the unprimed frame?* They must use $\psi'(\mathbf{r}')$ such that $\psi'(\mathbf{r}') = \psi(\mathbf{r})$ (compare the case of translations). Let's play with the algebra a bit:

$$\begin{aligned} \psi'(\mathbf{R}\mathbf{r}) &= \psi(\mathbf{r}) \\ \Rightarrow \psi'(\mathbf{r}) &= \psi(\mathbf{R}^{-1}\mathbf{r}) \quad . \end{aligned}$$

This little manipulation tells us what ψ' actually is. For instance in the case of $\mathbf{R} = \mathbf{R}_z(\alpha)$,

$$\begin{aligned} \psi'(x', y', z') &= \psi(x, y, z) \\ \Rightarrow \psi'(x \cos \alpha - y \sin \alpha, x \sin \alpha + y \cos \alpha, z) &= \psi(x, y, z) \\ \Rightarrow \psi'(x, y, z) &= \psi(x \cos \alpha + y \sin \alpha, -x \sin \alpha + y \cos \alpha, z) . \end{aligned}$$

For $\alpha \rightarrow \epsilon$ this means,

$$\begin{aligned} \psi'(x, y, z) &= \psi(x + \epsilon y, -\epsilon x + y, z) \\ \Rightarrow \psi'(x, y, z) &= \psi(x, y, z) + \epsilon y \frac{\partial \psi}{\partial x} - \epsilon x \frac{\partial \psi}{\partial y} \dots \\ \Rightarrow \psi'(x, y, z) &= \left(1 + \epsilon y \frac{\partial}{\partial x} + \epsilon x \frac{\partial}{\partial y} \right) \psi(x, y, z) \end{aligned}$$

$$\Rightarrow \psi'(x, y, z) = \left(1 - \frac{i\epsilon \hat{L}_z}{\hbar}\right) \psi(x, y, z),$$

where $\hat{L}_z = (\mathbf{r} \times \mathbf{p})_z = -i\hbar x \frac{\partial}{\partial y} + i\hbar y \frac{\partial}{\partial x}$ is the angular momentum operator for the z-component of angular momentum (because we have only considered rotations about the z-axis). So $\psi'(\mathbf{r}) = \left(1 - \frac{i\epsilon \hat{L}_z}{\hbar}\right) \psi(\mathbf{r})$ for this infinitesimal rotation. In words, what this important equation tells us is what we have to do to the function ψ (“operate on it with $\left(1 - \frac{i\epsilon \hat{L}_z}{\hbar}\right)$ ”) to produce ψ' - which is the answer to our question!

For a finite rotation about the z-axis we then have

$$\psi'(\mathbf{r}) = e^{-\frac{i\alpha \hat{L}_z}{\hbar}} \psi(\mathbf{r}).$$

For a general infinitesimal rotation,

$$\psi'(\mathbf{r}) = (1 - i\mathbf{a} \cdot \hat{\mathbf{L}}) \psi(\mathbf{r}) = (1 - i\epsilon \mathbf{n} \cdot \hat{\mathbf{L}}) \psi(\mathbf{r}),$$

and for a general finite rotation

$$\psi'(\mathbf{r}) = e^{-\frac{i\alpha \mathbf{n} \cdot \hat{\mathbf{L}}}{\hbar}} \psi(\mathbf{r})$$

(a rotation of α about the \mathbf{n} axis). We call $e^{-\frac{i\alpha \mathbf{n} \cdot \hat{\mathbf{L}}}{\hbar}}$ the rotation operator, denoted by $\hat{\mathbf{U}}_{\mathbf{R}}$, where \mathbf{R} is (in this case) the rotation by α about the axis \mathbf{n} . \hat{L}_z is the generator of rotations about the z-axis; the same goes for the x and y axes. So finally

$$\psi'(\mathbf{r}) = \hat{\mathbf{U}}_{\mathbf{R}} \psi(\mathbf{r})$$

tells us what the “primed” wavefunction is in terms of the unprimed one, and the rotation operator $\hat{\mathbf{U}}_{\mathbf{R}}$. Notice that both sides of all these last equations are evaluated at the same point \mathbf{r} .

Here a most important remark needs to be made: **the operator $\hat{\mathbf{U}}_{\mathbf{R}}$ is unitary, in the usual quantum-mechanical sense** i.e. $\hat{\mathbf{U}}_{\mathbf{R}}^\dagger \hat{\mathbf{U}}_{\mathbf{R}} = \mathbf{I}$. This is clearly needed in order to preserve the normalisation of ψ between the two frames. Note also how such $\hat{\mathbf{U}}$ ’s have the generic form “exponential of i times a Hermitian operator” where the “Hermitian operator” is a generator. Putting this another way, with such a unitary operator is associated a Hermitian generator of infinitesimal transformations which, precisely because it is Hermitian, is an *observable*. In this case, of course, the generators are the angular momentum operators.

The situation with rotations is “richer” than with translations. The generators of translations were $\hat{p}_x, \hat{p}_y, \hat{p}_z$ and these all commute; on the other hand the rotation generators $\hat{L}_x, \hat{L}_y, \hat{L}_z$ do not, as we all know, since they are just the angular momentum operators in quantum mechanics, with commutation relations

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk} \hat{L}_k.$$

This is known as the algebra of the generators of SO(3), or just as the SO(3) algebra, for short.

Just as in the case of translations, it may be the case that the Hamiltonian is invariant under the SO(3) transformation in which case

$$\hat{\mathbf{H}}'(\mathbf{r}) = \hat{\mathbf{U}}_{\mathbf{R}} \hat{\mathbf{H}}(\mathbf{r}) \hat{\mathbf{U}}_{\mathbf{R}}^{-1} = \hat{\mathbf{H}}(\mathbf{r}).$$

(Compare the similar thing for translations in the last lecture.) So if the Hamiltonian is invariant as above,

$$\hat{\mathbf{U}}_{\mathbf{R}} \hat{\mathbf{H}}(\mathbf{r}) = \hat{\mathbf{H}}(\mathbf{r}) \hat{\mathbf{U}}_{\mathbf{R}},$$

which requires that

$$[\hat{\mathbf{L}}, \hat{\mathbf{H}}] = 0.$$

So the eigenvalues of $\hat{\mathbf{L}}$ are constants of the motion, and “angular momentum is conserved”. But we cannot generally have states for which two or more components of $\hat{\mathbf{L}}$ all have well defined values because they don’t commute. However it is true that $\hat{\mathbf{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ commutes with any operator \hat{L}_i (where $i = x, y, z$). Usually the states are chosen to be eigenstates of $\hat{\mathbf{L}}^2$ and of \hat{L}_z , as well as of $\hat{\mathbf{H}}$.

We can imagine generalisations of the above state of affairs, in which the *Hermitian generators of some symmetry are observable conserved quantities - i.e. their eigenvalues are constants of the motion.*

Symmetry and Degeneracy.

We have:

$$\widehat{\mathbf{H}}(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}).$$

So

$$\widehat{\mathbf{U}}_{\mathbf{R}}\widehat{\mathbf{H}}(\mathbf{r})\widehat{\mathbf{U}}_{\mathbf{R}}^{-1}\widehat{\mathbf{U}}_{\mathbf{R}}\psi(\mathbf{r}) = \widehat{\mathbf{H}}'(\mathbf{r})\psi'(\mathbf{r}) = E\widehat{\mathbf{U}}_{\mathbf{R}}\psi(\mathbf{r}),$$

and if $\widehat{\mathbf{H}}'(\mathbf{r}) = \widehat{\mathbf{H}}(\mathbf{r})$ then

$$\widehat{\mathbf{H}}(\mathbf{r})\psi'(\mathbf{r}) = E\psi'(\mathbf{r}).$$

What this is saying is that $\psi'(\mathbf{r})$ has the same eigenvalue, E , of $\widehat{\mathbf{H}}(\mathbf{r})$ as $\psi(\mathbf{r})$ does. The conclusions we draw from this depend on whether the level E is degenerate or not:

- if E is non-degenerate then only one distinct wavefunction can belong to it and $\psi'(\mathbf{r})$ must be proportional to $\psi(\mathbf{r})$ (this proportionality factor can only be a phase factor, so as to preserve the probability density $|\psi(\mathbf{r})|^2$)
- if E is degenerate then several distinct “ $\psi(\mathbf{r})$ ’s” can have the same eigenvalue E . There will be the corresponding number of “ $\psi'(\mathbf{r})$ ’s”, and the “ $\psi'(\mathbf{r})$ ’s” will, in general, be linear superpositions of the “ $\psi(\mathbf{r})$ ’s”.

In the case where the level E is degenerate we need to distinguish the “different $\psi(\mathbf{r})$ ’s” by a label n , $\psi_n(\mathbf{r})$. Then any particular $\psi'_m(\mathbf{r})$ is a linear combination of the various $\psi_n(\mathbf{r})$ ’s:

$$\psi'_m(\mathbf{r}) = \sum_n D_{nm}(\mathbf{R})\psi_n(\mathbf{r}),$$

where $D_{nm}(\mathbf{R})$ is a matrix of coefficients for the $\psi_n(\mathbf{r})$ ’s, for the rotation \mathbf{R} . Note the order of the indices n, m on D_{nm} !

In Dirac notation $\psi_m(\mathbf{r}) = \langle \mathbf{r}|m\rangle$, while $\psi'_m(\mathbf{r}) = \widehat{\mathbf{U}}_{\mathbf{R}}\psi_m(\mathbf{r}) = \langle \mathbf{r}|\widehat{\mathbf{U}}_{\mathbf{R}}|m\rangle$. So

$$\langle \mathbf{r}|m'\rangle = \langle \mathbf{r}|\widehat{\mathbf{U}}_{\mathbf{R}}|m\rangle = \sum_n \langle \mathbf{r}|n\rangle \langle n|\widehat{\mathbf{U}}_{\mathbf{R}}|m\rangle$$

or, stripping away the $\langle \mathbf{r}|$ from everything,

$$|m'\rangle = \widehat{\mathbf{U}}_{\mathbf{R}}|m\rangle = \sum_n |n\rangle \langle n|\widehat{\mathbf{U}}_{\mathbf{R}}|m\rangle = \sum_n D_{nm}(\mathbf{R})|n\rangle.$$

The superposition coefficients $D_{nm}(\mathbf{R})$ are just the matrix elements of the rotation operator $\widehat{\mathbf{U}}_{\mathbf{R}}$ in the basis $\{|n\rangle\}$.

Another important remark comes here: these \mathbf{D} matrices are unitary matrices, just as the operators $\widehat{\mathbf{U}}_{\mathbf{R}}$ (whose matrix elements they are) are unitary operators. [Exercise: prove the \mathbf{D} ’s are unitary!]

Consider now two rotations, first \mathbf{R} then \mathbf{S} i.e. \mathbf{SR} . What is the corresponding $D_{nm}(\mathbf{SR})$? Under “first R , then S ”,

$$\psi_m(\mathbf{r}) \rightarrow \psi'_m(\mathbf{r}) = \widehat{\mathbf{U}}_{\mathbf{S}}\widehat{\mathbf{U}}_{\mathbf{R}}\psi_m(\mathbf{r}),$$

hence we define $\widehat{\mathbf{U}}_{\mathbf{SR}} = \widehat{\mathbf{U}}_{\mathbf{S}}\widehat{\mathbf{U}}_{\mathbf{R}}$, and

$$\psi'_m(\mathbf{r}) = \widehat{\mathbf{U}}_{\mathbf{SR}}\psi_m(\mathbf{r}) = \widehat{\mathbf{U}}_{\mathbf{S}}\widehat{\mathbf{U}}_{\mathbf{R}}\psi_m(\mathbf{r}) = \widehat{\mathbf{U}}_{\mathbf{S}} \left(\sum_n D_{nm}(\mathbf{R})\psi_n(\mathbf{r}) \right).$$

As the \mathbf{D} ’s are just numbers we can bring the $\widehat{\mathbf{U}}_{\mathbf{S}}$ operator inside the summation as follows,

$$\begin{aligned} \psi'_m(\mathbf{r}) &= \sum_n D_{nm}(\mathbf{R}) \left(\widehat{\mathbf{U}}_{\mathbf{S}}\psi_n(\mathbf{r}) \right) = \sum_n D_{nm}(\mathbf{R}) \left(\sum_p D_{pn}(\mathbf{S})\psi_p \right) \\ &\Rightarrow \psi'_m(\mathbf{r}) = \widehat{\mathbf{U}}_{\mathbf{SR}}\psi_m(\mathbf{r}) = \sum_p \left(\sum_n D_{pn}(\mathbf{S})D_{nm}(\mathbf{R}) \right) \psi_p(\mathbf{r}). \end{aligned}$$

The left hand side of the above equation is also, by definition,

$$\widehat{\mathbf{U}}_{\mathbf{SR}}\psi_m(\mathbf{r}) = \sum_p D_{pm}(\mathbf{SR})\psi_p(\mathbf{r}).$$

Comparing this to the previous equation we see that:

$$D_{pm}(\mathbf{SR}) = \sum_n D_{pn}(\mathbf{S})D_{nm}(\mathbf{R}).$$

The right hand side is just matrix multiplication! So the \mathbf{D} matrices multiply together in exactly the same way as the rotation group elements $\mathbf{R}, \mathbf{S}, \dots$ (which is obviously the same way as the operators $\widehat{\mathbf{U}}_{\mathbf{R}}, \widehat{\mathbf{U}}_{\mathbf{S}}, \dots$). This being the case the \mathbf{D} matrices are said to form a matrix representation of the group SO(3). The degenerate wavefunctions $\psi_m(\mathbf{r})$ are said to form a basis for this representation. If the number of degenerate states is d , then the \mathbf{D} 's are $d \times d$ matrices and the representation is said to be d-dimensional. Incidentally, people sometimes get momentarily puzzled by the fact that what the matrices \mathbf{D} are representing are the elements of SO(3), which are themselves matrices.... It's OK. All we are saying is that there are lots of other matrices that multiply together the same way that the SO(3) matrices do. It is pretty amazing, all the same!

Example:

Suppose we have three degenerate states (our basis), $\psi_1(\mathbf{r}) = x$, $\psi_2(\mathbf{r}) = y$, $\psi_3(\mathbf{r}) = z$. Consider a rotation $\mathbf{R}_z(\alpha)$.

$$\begin{aligned} \psi'_m(\mathbf{r}') &= \psi_m(\mathbf{r}) \\ \psi'_m(\mathbf{R}_z(\alpha)\mathbf{r}) &= \psi_m(\mathbf{r}) \\ \psi'_m(\mathbf{r}) &= \psi_m(\mathbf{R}_z^{-1}(\alpha)\mathbf{r}) \\ \Rightarrow \psi'_m(\mathbf{r}) &= \psi_m(x \cos \alpha + y \sin \alpha, -x \sin \alpha + y \cos \alpha, z). \end{aligned}$$

The function $\psi_1(\mathbf{r})$ is just x , i.e. the function ψ_1 simply “returns” the first component of its vector argument. So

$$\psi'_1(\mathbf{r}) = \psi_1(x \cos \alpha + y \sin \alpha, -x \sin \alpha + y \cos \alpha, z) = x \cos \alpha + y \sin \alpha$$

which we can write as

$$\psi'_1(\mathbf{r}) = \psi_1(\mathbf{r}) \cos \alpha + \psi_2(\mathbf{r}) \sin \alpha = \sum_m D_{m1}(\mathbf{R}_z(\alpha))\psi_m(\mathbf{r})$$

and then read off

$$D_{11}(\mathbf{R}_z(\alpha)) = \cos \alpha, \quad D_{21}(\mathbf{R}_z(\alpha)) = \sin \alpha, \quad D_{31}(\mathbf{R}_z(\alpha)) = 0.$$

By considering $\psi_2(\mathbf{r})$ and $\psi_3(\mathbf{r})$ in the same way, we can find $D_{12}, D_{22}, D_{32}, D_{13}, D_{23}, D_{33}$. These all form the elements of a particular \mathbf{D} matrix:

$$\mathbf{D}^{(1)}(\mathbf{R}_z(\alpha)) = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Note that this $\mathbf{D}^{(1)}$ is entirely real, so rather than being unitary it is *orthogonal* i.e. in SO(3) - in fact, it is actually $\mathbf{R}_z(\alpha)$ itself! (not really surprising considering our basis functions are $\psi_1(\mathbf{r}) = x$, $\psi_2(\mathbf{r}) = y$, $\psi_3(\mathbf{r}) = z$, and we started by considering transformations of the vector \mathbf{r}).

By considering infinitesimal transformations ($\cos \alpha \rightarrow 1$, $\sin \alpha \rightarrow \epsilon$) we can get a matrix representation for the generator \widehat{L}_z :

$$\mathbf{D}^{(1)}(\mathbf{R}_z(\epsilon)) = \begin{pmatrix} 1 & -\epsilon & 0 \\ \epsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = 1 - \frac{i\epsilon L_z^{(1)}}{\hbar},$$

where

$$L_z^{(1)} = \hbar \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The “ $^{(1)}$ ” stands for “ $l = 1$ ” because the three basis wavefunctions are (as far as rotations are concerned) the same as (linear combinations of) p-state wavefunctions; we shall not put hats on symbols standing for matrices - they represent

the things with hats on, in a particular basis. By considering rotations about the x-axis and y-axis, we can similarly find:

$$L_x^{(1)} = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \text{ and } L_y^{(1)} = \hbar \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix},$$

where

$$[L_x^{(1)}, L_y^{(1)}] = i\hbar L_z^{(1)}.$$

So the required commutation relations (of the $\text{SO}(3)$ algebra) are satisfied by this matrix representation of the algebra of the generators of $\text{SO}(3)$ (or just “matrix representation of the generators of $\text{SO}(3)$ ”), with dimension $d=3$ (3×3 matrices). It is an interesting exercise to check that for the finite rotation case, the matrix $\mathbf{D}^{(1)}(\mathbf{R}_z(\alpha))$ can be written as $e^{-i\alpha L_z^{(1)}}$ (compare the similar result with 2×2 matrices in the next lecture).