Finding representations of the symmetry group of a square using its modes

There are 8 elements of the group of symmetry of the square:

- E – identity
- C_4, C_4^3 – rotations by $\pm\pi/2$
- C_2 – rotation by π
- σ_x – reflection in the horizontal axis
- σ_y – reflection in the vertical axis
- ρ_1 – reflection in the "main diagonal"
- ρ_2 – reflection in the "other diagonal"

It turns out that these elements fall into five conjugacy classes like this:

$$\{E\},\ \{C_2\},\ \{C_4, C_4^3\},\ \{\sigma_x, \sigma_y\},\ \{\rho_1, \rho_2\}.$$

1 Modes

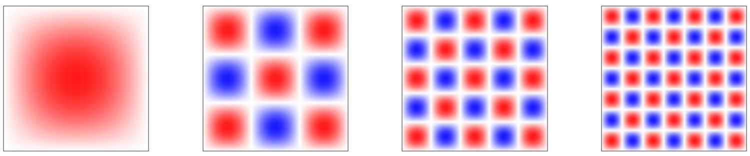
The modes of a unit square are $\psi_{mn}(x, y) = \sin(m\pi x)\sin(n\pi y)$ (we do not worry about normalisation factors now) and they can be seen in Fig. 1. Let us look at their representations.

2 Non-degenerate modes

The non-degenerate modes are ψ_{nn}. They can be separated into two categories.

2.1 Odd n

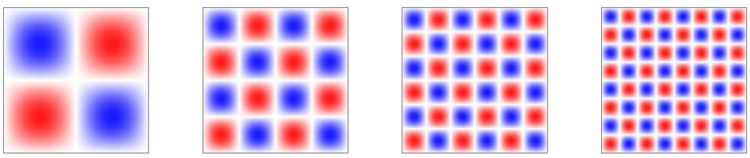
First consider the modes with an odd n:



Clearly, all group elements leave them completely identical, therefore we get the representation where all elements are assigned the unit matrix, (1).

2.2 Even n

Second, consider the modes with even n:



We easily get the representation table:

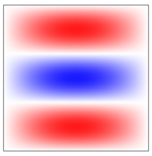
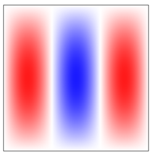
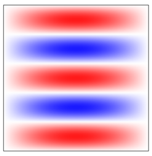
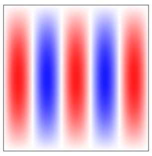
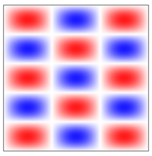
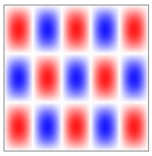
E	C_4	C_4^3	C_2	σ_x	σ_y	ρ_1	ρ_2
(1)	(−1)	(−1)	(1)	(−1)	(−1)	(1)	(1)

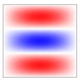
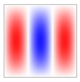
3 Degenerate modes

The degenerate modes are ψ_{mn} and can be divided into four categories, depending on the parity of the numbers m, n.

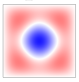
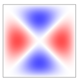
3.1 Both m, n odd

First consider the modes with both m, n odd:

Taking an example of $m = 1, n = 3$, we have the basis functions  and . It is easy to work out the representation as follows:

E	C_4	C_4^3	C_2	σ_x	σ_y	ρ_1	ρ_2
$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$

We can also work in a different basis instead, namely $\phi_{mn} = (\psi_{mn} + \psi_{nm})/\sqrt{2}$, $\xi_{mn} = (\psi_{mn} - \psi_{nm})/\sqrt{2}$, which corresponds to the basis functions shown in Figs. 2 and 3. For the example of $m = 1, n = 3$, the modes are  and . Then all the representation matrices change too; the new matrices are related to the original ones by a similarity transformation

$$M_{\text{new}} = S M_{\text{old}} S^{-1} \qquad \text{with} \qquad S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

This leads to new representation matrices

E	C_4	C_4^3	C_2	σ_x	σ_y	ρ_1	ρ_2
$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$

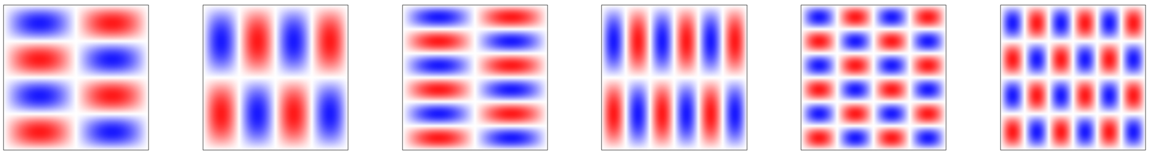
We see that all these matrices are now diagonal, with 1 at position $_{11}$ and ± 1 at position $_{22}$. This means that the mode ϕ_{mn} transforms always to itself and the mode ξ_{mn} transforms to itself up to a possible sign flip. This also means that the representation is *reducible* and can be composed (written as a direct sum) of 1D representations. Clearly, the elements at positions $_{11}$ correspond to the trivial representation discussed in Sec. 2.1. The elements at position $_{22}$ produce a new 1D representation:

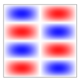
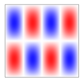
E	C_4	C_4^3	C_2	σ_x	σ_y	ρ_1	ρ_2
(1)	(-1)	(-1)	(1)	(1)	(1)	(-1)	(-1)

The fact that the 2D representation separates in two 1D representations means that if we modify the Hamiltonian slightly, keeping the symmetry of the square, the degeneracy might be removed and the modes would be separated. It is not hard to find the change needed for that. In particular, adding a Dirac δ potential at the centre fo the square would change the energy of the mode ϕ_{mn} but not that of ξ_{mn}, so the degeneracy would be removed.

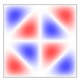
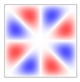
3.2 Both m, n even

Next consider the modes with both m, n even:



The representation using the basis functions  and  is as follows:

E	C_4	C_4^3	C_2	σ_x	σ_y	ρ_1	ρ_2
$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix} & -1\\ -1 & \end{pmatrix}$	$\begin{pmatrix} & -1\\ -1 & \end{pmatrix}$	$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}-1 & \\ & -1\end{pmatrix}$	$\begin{pmatrix}-1 & \\ & -1\end{pmatrix}$	$\begin{pmatrix} & 1\\ 1 & \end{pmatrix}$	$\begin{pmatrix} & 1\\ 1 & \end{pmatrix}$

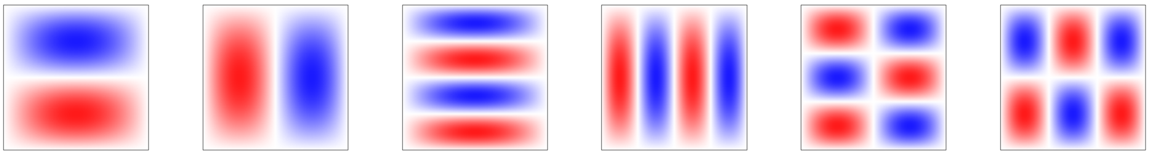
However, the representation using the alternative basis functions  and  is as follows:

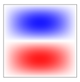
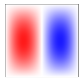
E	C_4	C_4^3	C_2	σ_x	σ_y	ρ_1	ρ_2
$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}-1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}-1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}-1 & \\ & -1\end{pmatrix}$	$\begin{pmatrix}-1 & \\ & -1\end{pmatrix}$	$\begin{pmatrix}1 & \\ & -1\end{pmatrix}$	$\begin{pmatrix}1 & \\ & -1\end{pmatrix}$

We see that again the representation is reducible, giving rise to two additional 1D representations. Again, we can ask how to modify the Hamiltonian, keeping the symmetry of the square, to remove the degeneracy. Imagine we add an infinitely high potential barrier in the form of a circle around the square centre. This would influence the modes ϕ_{mn} more than ξ_{mn}, raising the energy, so the degeneracy would be removed.

3.3 One of the m, n odd, the other one even

Next consider the modes with one of the m, n odd, the other one even:



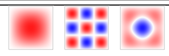
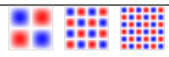
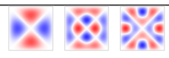
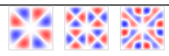
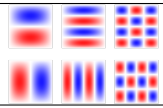
The representation using the basis functions  and  is as follows:

E	C_4	C_4^3	C_2	σ_x	σ_y	ρ_1	ρ_2
$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix} & 1\\ -1 & \end{pmatrix}$	$\begin{pmatrix} & -1\\ 1 & \end{pmatrix}$	$\begin{pmatrix}-1 & \\ & -1\end{pmatrix}$	$\begin{pmatrix}-1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}1 & \\ & -1\end{pmatrix}$	$\begin{pmatrix} & -1\\ -1 & \end{pmatrix}$	$\begin{pmatrix} & 1\\ 1 & \end{pmatrix}$

Using a different basis does not help to reduce this representation, so it is irreducible.

4 Table of all irreducible representations

Putting everything together, we arrive at the table of all irreducible representations of the symmetry group of the square. Four of them are 1D and one is 2D:

E	C_4	C_4^3	C_2	σ_x	σ_y	ρ_1	ρ_2	examples
(1)	(1)	(1)	(1)	(1)	(1)	(1)	(1)	
(1)	(-1)	(-1)	(1)	(-1)	(-1)	(1)	(1)	
(1)	(-1)	(-1)	(1)	(1)	(1)	(-1)	(-1)	
(1)	(1)	(1)	(1)	(-1)	(-1)	(-1)	(-1)	
$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix} & 1\\ -1 & \end{pmatrix}$	$\begin{pmatrix} & -1\\ 1 & \end{pmatrix}$	$\begin{pmatrix}-1 & \\ & -1\end{pmatrix}$	$\begin{pmatrix}-1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}1 & \\ & -1\end{pmatrix}$	$\begin{pmatrix} & -1\\ -1 & \end{pmatrix}$	$\begin{pmatrix} & 1\\ 1 & \end{pmatrix}$	

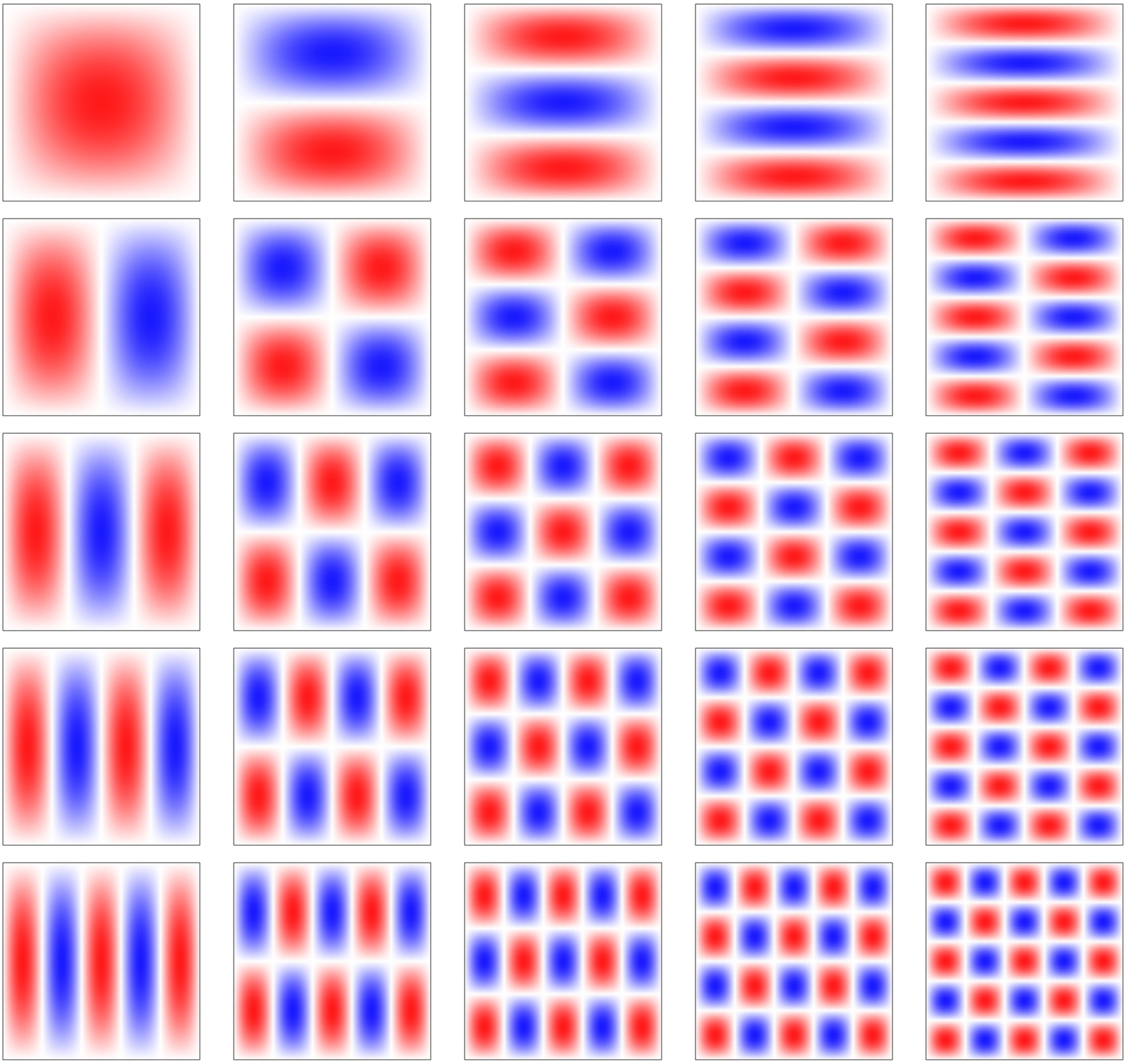


Figure 1: Modes of the unit square with corners $[0,0]$ and $[1,1]$ in the form $\psi_{mn}(x,y) = \sin(m\pi x)\sin(n\pi y)$ for m,n ranging from 1 to 5.

5 Characters

In the preceding text we saw that some of the two-dimensional representations (the ones shown in Secs. 3.1 and 3.2) were in fact *reducible*: they were made up of smaller representations. We managed to detect this because of a fortunate change of basis. However, just trying different bases and hoping for the modes to decouple is a terrible way of testing the reducibility. Obviously we would like to have a better tool for this, and the tool should ideally be something that is independent of choice of a basis.

There are several such invariants in linear algebra, but the one that will turn out to be really useful is the trace. First we need to realize that in a trace of a product, $\mathrm{Tr}[M_1 M_2 \cdots M_n]$, we may permute the factors cyclically (i. e. move the last one to the front, or the first one to the back) and the trace is not changed. If we take a matrix M and use another matrix S to change to a different basis, we find that the trace of the new matrix is

$$\mathrm{Tr}[SMS^{-1}] = \mathrm{Tr}[S^{-1}SM] = \mathrm{Tr}\, M,$$

i. e. the trace is truly invariant with respect to the change of basis. These traces are so useful that they get a special name: *characters*. They're most often denoted by the Greek letter χ.

The characters have another important property: if an element g has a character $\chi(g)$, then any element conjugate to it, let's say hgh^{-1}, has the character equal to $\mathrm{Tr}[D(hgh^{-1})]$ (D is the representation matrix for the given element). The representation matrices must still obey the same laws of multiplication as the group elements, so we get that

$$\chi(hgh^{-1}) = \mathrm{Tr}[D(hgh^{-1})] = \mathrm{Tr}[D(h)D(g)D(h)^{-1}] = \mathrm{Tr}[D(h)^{-1}D(h)D(g)] = \mathrm{Tr}\, D(g) = \chi(g),$$

and *all elements in the same conjugation class have the same character.*

Now we can assemble a table similar to the table in Sec. 4. The only differences will be that instead of 8 columns, one for each element, only five will suffice (one for each conjugacy class — see the beginning), and instead of the matrices, we write their traces. We obtain the following result:

No.	E	$2C_4$	C_4^2	2σ	2ρ
I	1	1	1	1	1
II	1	−1	1	−1	1
III	1	−1	1	1	−1
IV	1	1	1	−1	−1
V	2	0	−2	0	0

For our purposes, I just denoted the irreducible representations by some Roman numerals, although it is customary to give them other names. As for the column headings: for instance, the column $2C_4$ means that it gives the character for the whole conjugacy class of C_4 rotations, and the 2 in front means there are two elements in that class. Some tables prefer to write $C_4\,(2)$ or something similar.

So what use will those characters be to us? They have a very powerful property that we will not prove right now: they are *orthogonal*. By that I mean the following: if we consider each row to be a vector with 8 components and perform the usual "dot product" with two different rows (i. e. if we add the products of the corresponding components), we get a zero. For instance, making such a dot product between rows I and II gives

$$\boldsymbol{\chi}_I \cdot \boldsymbol{\chi}_{II} = 1 \cdot 1 + 2 \cdot 1 \cdot (-1) + 1 \cdot 1 + 2 \cdot 1 \cdot (-1) + 2 \cdot 1 \cdot 1 = 1 - 2 + 1 - 2 + 2 = 0.$$

Observe that we multiply the characters element-by-element, so for instance the product of the column "$2C_4$" must be taken twice — it actually shows characters for two elements at the same time.

On the other hand, if we make a dot product of characters of an irreducible representation with themselves, we get the order of the group (in our case, 8). In the case of rows I–IV, it is obvious (we add up 8 squares of ± 1). For the row V, we calculate $2^2 + (-2)^2 + \text{some zeroes} = 8$.

What does that mean for a compound representation like the one in Sec. 3.1? We saw that such a representation is given by block-diagonal matrices (in some appropriate basis), and the blocks are just the matrices of the irreducible representations out of which the compound representation is made. Obviously the trace of such a matrix is just the sum of the traces of the blocks, and so the character of the compound representation is just the sum of the irreducible characters.

Now let's see what happens for a representation built out of two different irreducible representations with characters $\boldsymbol{\chi}_1$ and $\boldsymbol{\chi}_2$. Its character will be simply $\boldsymbol{\chi}_1 + \boldsymbol{\chi}_2$. What happens when we take a dot product of this with itself? We get

$$(\boldsymbol{\chi}_1 + \boldsymbol{\chi}_2)^2 = \boldsymbol{\chi}_1^2 + 2\boldsymbol{\chi}_1 \cdot \boldsymbol{\chi}_2 + \boldsymbol{\chi}_2^2.$$

Both squares equal to 8, and if the two representations are different, their characters are orthogonal, which means that the cross-term in the middle vanishes. Hence the result will be 16. On the other hand: what happens if the representation is built out of two copies of the same representation $\boldsymbol{\chi}_1$? Then the dot product of the character $2\boldsymbol{\chi}_1$ with itself will be $4\boldsymbol{\chi}_1^2 = 32$.

Considerations like that show the following: if a representation is built out of n_1 copies of one irreducible representation, n_2 copies of another, and so on, the dot product of its character with itself will be $(n_1^2 + n_2^2 + \cdots) \cdot |G|$.

So now let's look at the two-dimensional representations in Sec. 3.1 and 3.2. Let's take the traces of the matrices. We find the following:

	E	$2C_4$	C_4^2	2σ	2ρ
both odd	2	0	2	2	0
both even	2	0	2	−2	0

Taking the dot product of each row with itself, we find that the result is 16 in both cases. How can we write 16 as a product of 8 and a sum of squares of some positive integers? There is only one way: $16 = 8 \cdot (1^2 + 1^2)$. We immediately see that both of these representations are made of two irreducible ones, each in one copy.

Can we find what irreducible representations they are, exactly? Yes! Orthogonality is still the key. If we take the compound character $\boldsymbol{\chi}_1 + \boldsymbol{\chi}_2$ and take a dot product with, for instance, $\boldsymbol{\chi}_1$, we find that the result is $\boldsymbol{\chi}_1^2 + \boldsymbol{\chi}_1 \cdot \boldsymbol{\chi}_2 = 8 + 0 = 8$, and we see there is one copy of it. If, on the other hand, we multiply the compound character with another character not contained in it, we get $0 + 0 = 0$.

Let's try that with the "both odd" representation. Take a dot product of its characters with characters of irreducible representation I. We get:

$$2 \cdot 1 + 2 \cdot 0 \cdot 1 + 2 \cdot 1 + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot 1 = 2 + 2 + 4 = 8.$$

So the representation I is present in one copy. Is there any copy of representation II? Let's take the dot product:

$$2 \cdot 1 + 2 \cdot 0 \cdot (-1) + 2 \cdot 1 + 2 \cdot 2 \cdot (-1) + 2 \cdot 0 \cdot 1 = 2 + 2 - 4 = 0.$$

No, there is no copy of that. Is there any copy of III?

$$2 \cdot 1 + 2 \cdot 0 \cdot (-1) + 2 \cdot 1 + 2 \cdot 2 \cdot 1 + 2 \cdot 0 \cdot (-1) = 2 + 2 + 4 = 8.$$

Yes, there is one copy. In fact, we are done, because the representation in question was two-dimensional and we already found two one-dimensional pieces contained in it. So there cannot be any more. If you go back to Sec. 3.1, you will find that this is exactly what we found there.

The pattern should be quite clear now. I invite you to try the same with the "both even" representation. You should find that it is made of irreducible representations II and IV, each in one copy.

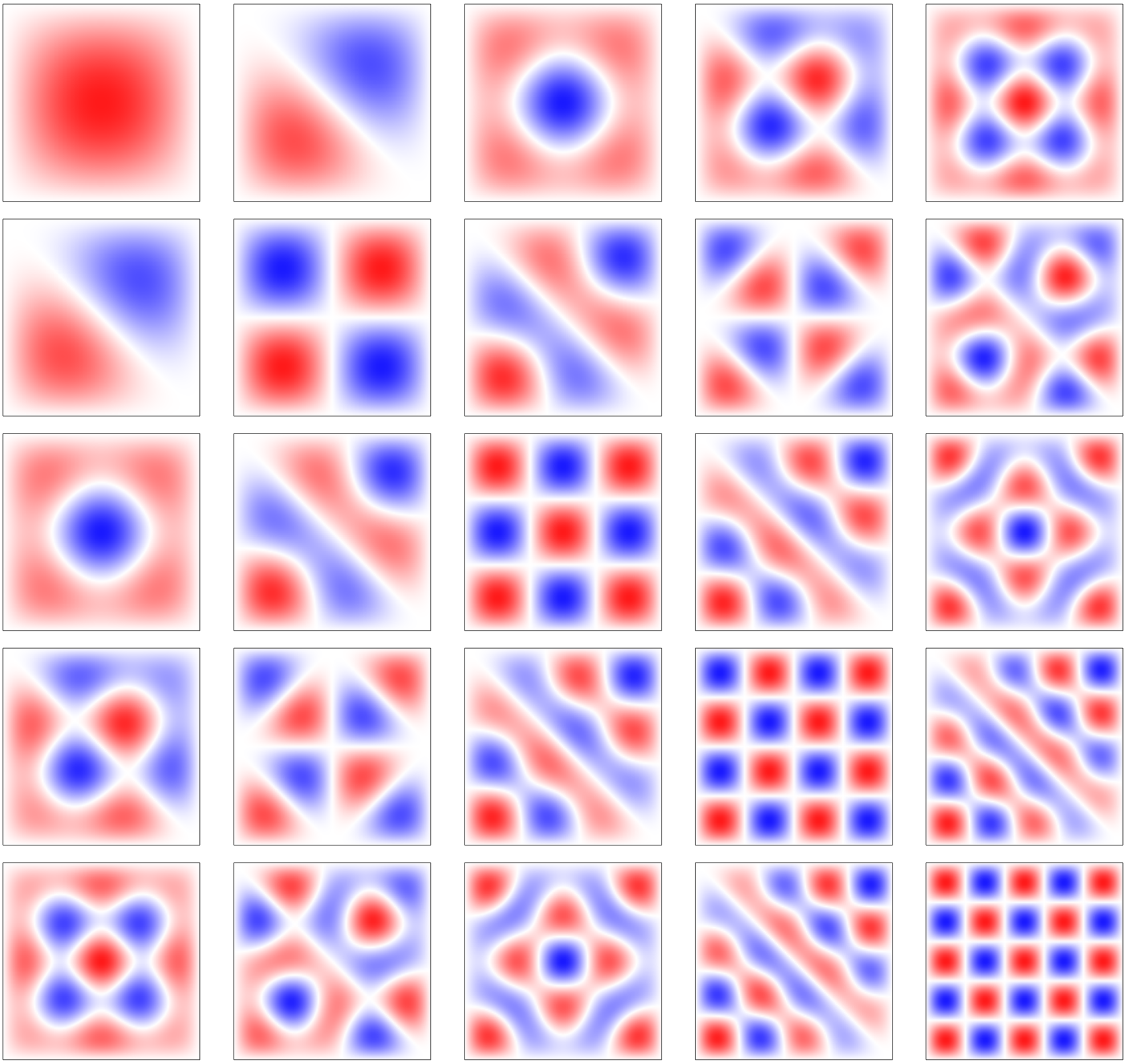


Figure 2: Modes of the unit square with corners [0, 0] and [1, 1] in the form $\phi_{mn} = (\psi_{mn} + \psi_{nm})/\sqrt{2}$.

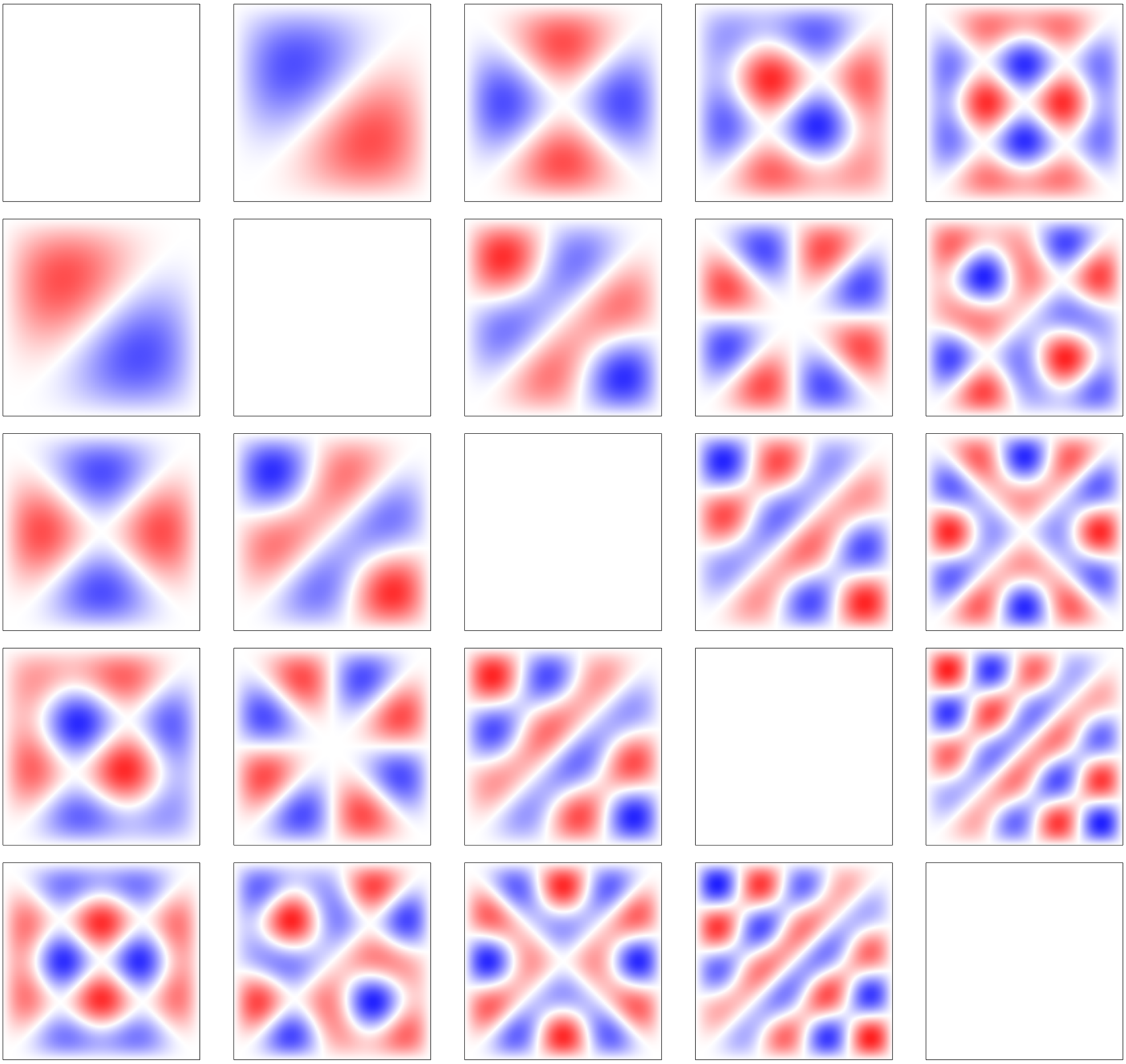


Figure 3: Modes of the unit square with corners [0, 0] and [1, 1] in the form $\xi_{mn} = (\psi_{mn} - \psi_{nm})/\sqrt{2}$.