Modes on cube

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Statement of the problem

We try to (surprise!) find modes on the cube.

That means that we want to solve the Schrödinger equation on it: $\mathcal{H}\psi = E\psi$. Here $\mathcal{H} = -\frac{1}{2}\,\Delta\,\psi$, so we have the Helmholtz equation:

$$\Delta\psi + 2E\psi = 0.$$

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The problem is that solutions are known only for a couple of domains (square, certain special triangles, sphere etc.) And the cube is not one of them.

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We describe the symmetry of the cube with group theory. It turns out that we can extract enough info from it to get the full solution of the problem.

How representations help

Let's have any Hamiltonian $\mathcal{H}$ that is invariant with respect to some operations g forming a group G. That means that $g\mathcal{H}g^{-1} = \mathcal{H}$.

Take Schrödinger equation $\mathcal{H}\psi = E\psi$. Multiply with g on the left, and insert $g^{-1}g = 1$ in the indicated place to get

$$g\mathcal{H}g^{-1}g\psi = Eg\psi \qquad \Longrightarrow \qquad \mathcal{H}g\psi = Eg\psi.$$

So if ψ is an eigenstate with energy E, $g\psi$ is also an eigenstate with the same E.

Symmetries of the cube

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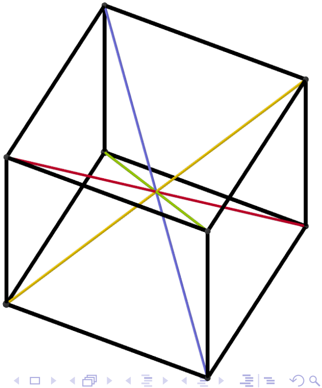
First, let's look at the rotations. There are $6 \times 4 = 24$ rotations that don't change the cube. The group of these rotations is S_4, which can be shown using a clever argument.

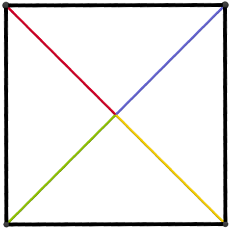


Rotations of the cube

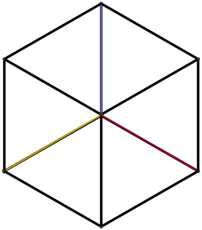
If we color-code the four body diagonals of the cube, we find that there is a 1:1 correspondence between each of the 24 rotations and the permutations of the four diagonals:

C_4	One 4-cycle	$3 \times 2 = 6$ pcs
C_3	One 3-cycle	$4 \times 2 = 8$ pcs
C_4^2	Product of two 2-cycles	3 pcs
C_2	One 2-cycle	6 pcs
Identity	()	1 pc
Total		**24 pcs**

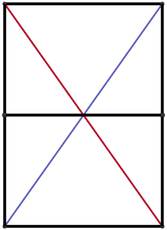
Rotations of the cube graphically



C_4 axis



C_3 axis



C_2 axis

Full cube group

Adding reflections, we get the full group of cube symmetries, $S_4 \times \mathbb{Z}_2$, also called the *octahedral group*.

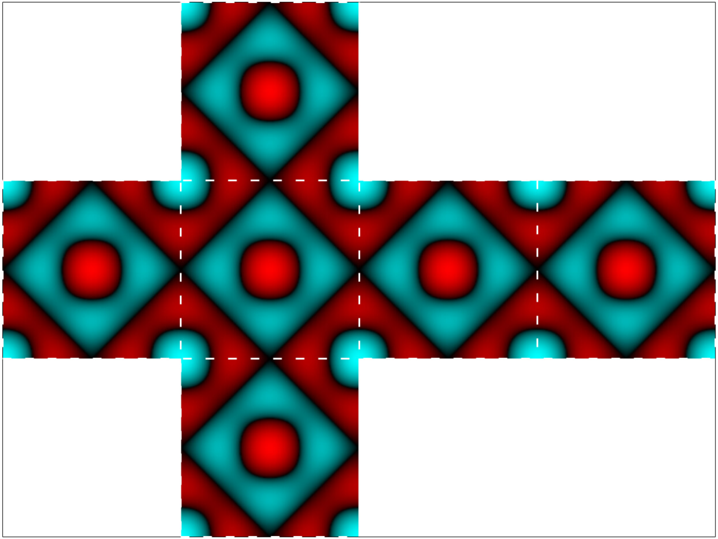
Now we can obtain all the irreducible representations for this group. There are 10 of them, as summarized in a so-called *character table*.

Character table

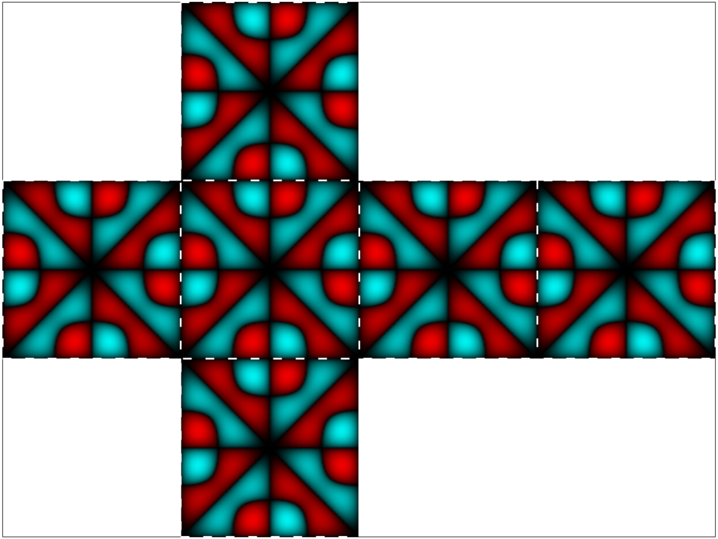
	$\mathbb{1}$	$8\,C_3$	$6\,C_2$	$6\,C_4$	$3\,C_4^2$	R	$6\,S_4$	$8\,S_6$	$3\,\sigma_h$	$6\,\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	−1	−1	1	1	−1	1	1	−1
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
A_{2u}	1	1	−1	−1	1	−1	1	−1	−1	1
E_g	2	−1	0	0	2	2	0	−1	2	0
E_u	2	−1	0	0	2	−2	0	1	−2	0
T_{1g}	3	0	−1	1	−1	3	1	0	−1	−1
T_{2g}	3	0	1	−1	−1	3	−1	0	−1	1
T_{1u}	3	0	−1	1	−1	−3	−1	0	1	1
T_{2u}	3	0	1	−1	−1	−3	1	0	1	−1

Non-degenerate

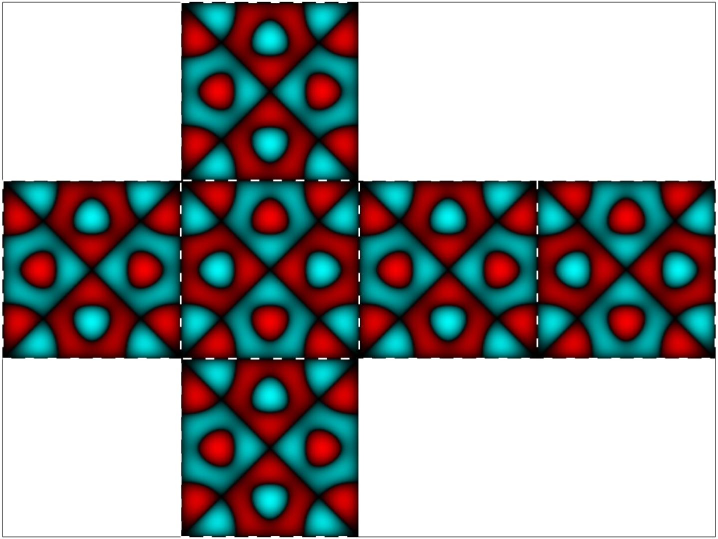
A_{1g}



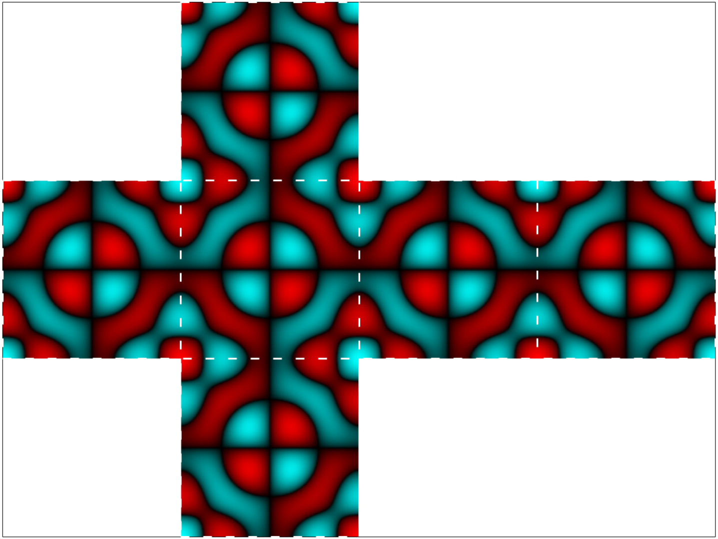
A_{1u}



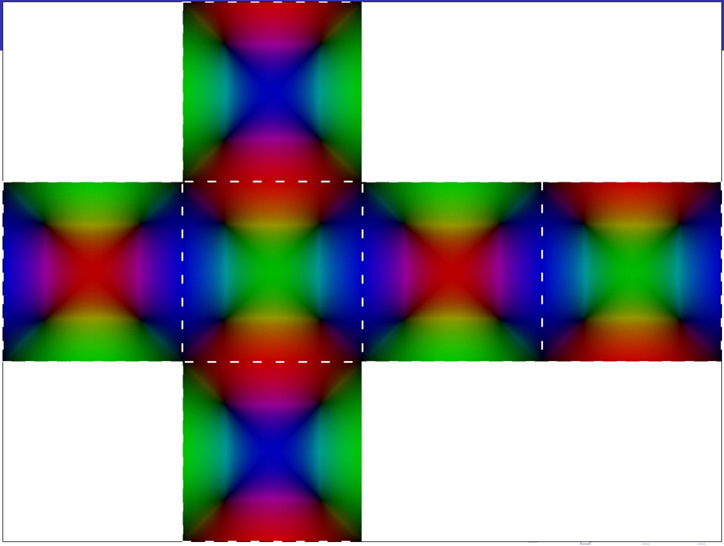
A_{2g}



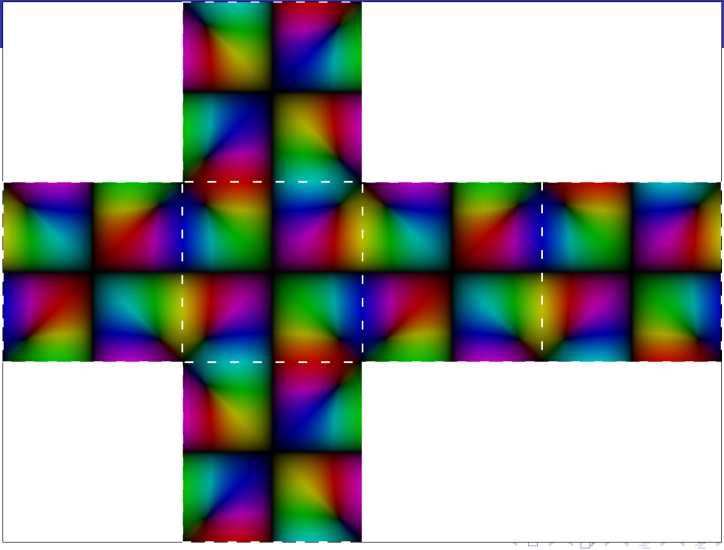
A_{2u}



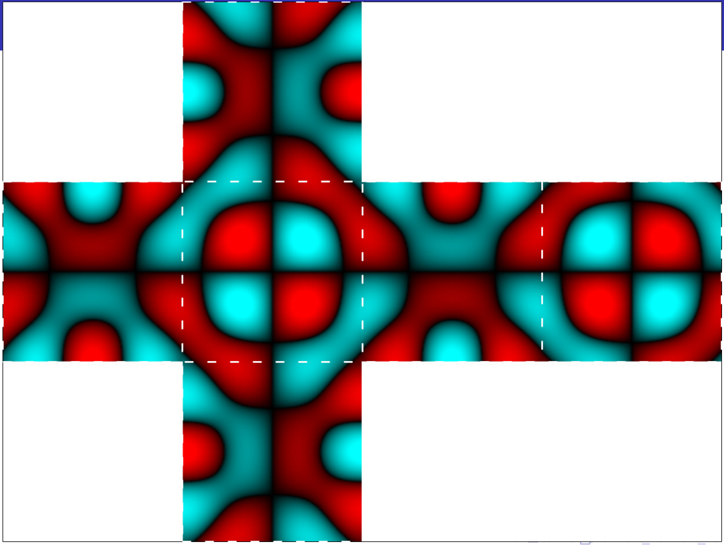
E_g



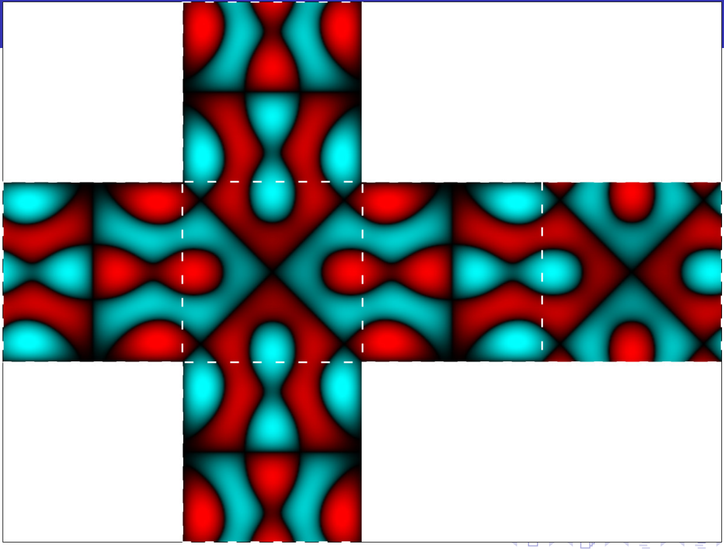
E_u



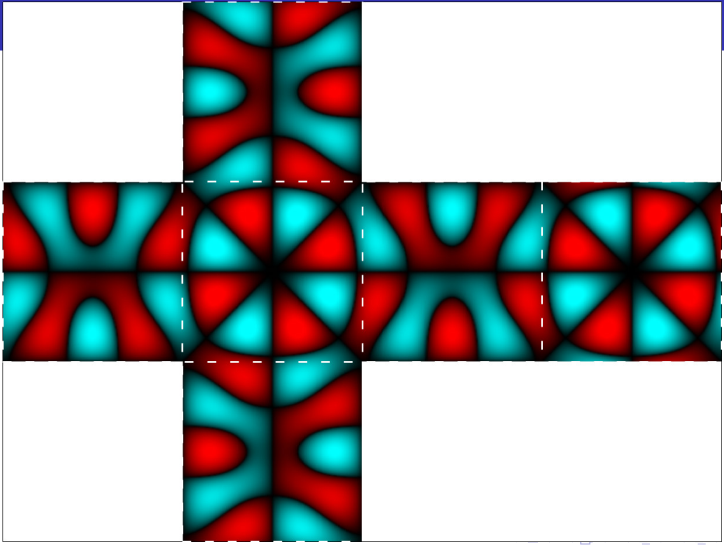
T_{1g}



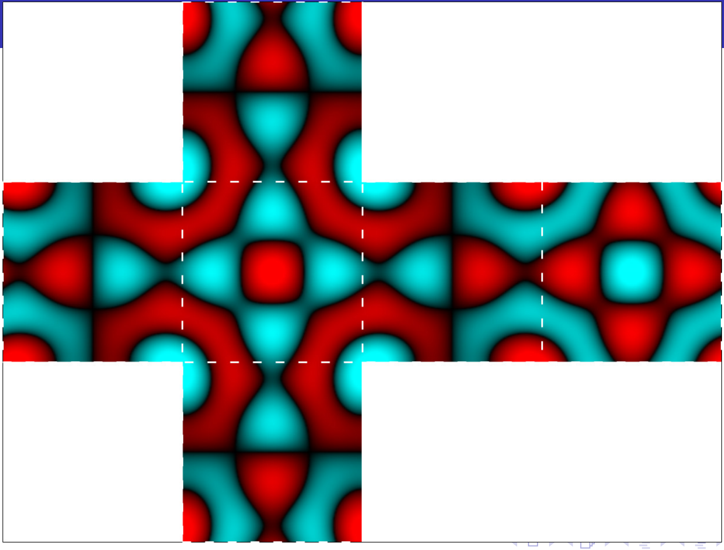
T_{1u}



T_{2g}

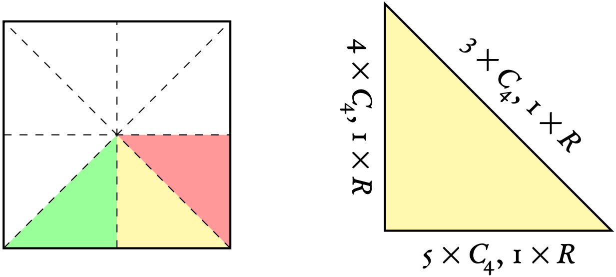


T_{2u}



Simplifying the problem

These representations tell us how the modes change when we perform any of the 48 symmetry operations. Hence it suffices to solve the problem on $\frac{1}{48}$ of the cube (= $\frac{1}{8}$ of a face).



We call this little triangle the *fundamental domain*.

Boundary conditions for non-degenerate modes

So we need to solve $\Delta\psi + 2E\psi = 0$ on one of the little triangles only. However, that will need some boundary conditions. These can be obtained with a simple lemma. For the non-degenerate modes it is almost trivial:

Lemma. *If the reflection through a straight line segment results in a function getting multiplied by λ, then:*

1. *If $\lambda = 1$, the normal derivative is zero at the segment.*
2. *If $\lambda \neq 1$, the function itself is zero at the segment.*

Boundary conditions for degenerate modes

For the degenerate modes, the reflection through a side of the fundamental domain results in the modes getting shuffled by a matrix. Then the lemma gets a bit more complicated:

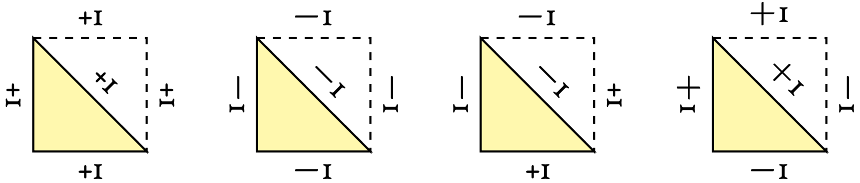
Better Lemma. *Let $f_1, f_2, \ldots, f_n$ be a basis and $\psi = c^k f_k$. If the reflection through a straight line changes the basis f_k to $\mathcal{M}_k^\ell f_\ell$, then:*

1. *ψ at the segment must be an eigenvector of $\mathcal{M}$ with eigenvalue of 1.*
2. *The normal derivative of ψ at the segment must be an eigenvector of $\mathcal{M}$ with eigenvalue of -1.*

Boundary conditions for non-degenerate modes

Let's put our lemma to work. The modes will behave like this:

A_{1g}	A_{1u}	A_{2g}	A_{2u}



Explicit formulas for non-degenerate modes

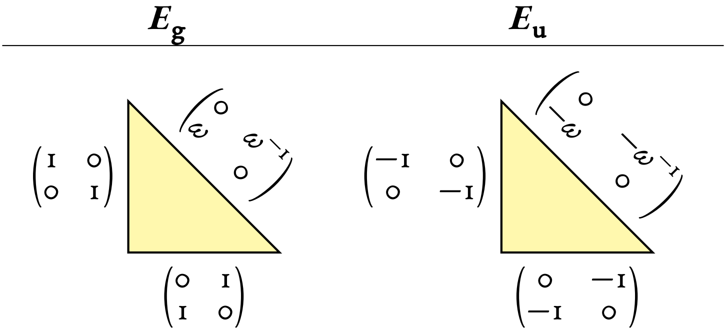
Now we must solve the Helmholtz equation on the square with the additional boundary conditions given by the lemma. That's textbook stuff. We obtain the results:

Explicit formulas for non-degenerate modes

A_{1g}	$\cos\pi kx\cos\pi\ell y+(-1)^{k+\ell}\cos\pi ky\cos\pi\ell x$ $E=\frac{1}{2}\pi^2(k^2+\ell^2)$
A_{1u}	$\sin\pi kx\sin\pi\ell y-(-1)^{k+\ell}\sin\pi ky\sin\pi\ell x$ $E=\frac{1}{2}\pi^2(k^2+\ell^2)$
A_{2g}	$\sin\pi\frac{2k+1}{2}x\cos\pi\frac{2\ell+1}{2}y-(-1)^{k+\ell}\sin\pi\frac{2\ell+1}{2}x\cos\pi\frac{2k+1}{2}y$ $E=\frac{\pi^2}{2}\left[\left(\frac{2k+1}{2}\right)^2+\left(\frac{2\ell+1}{2}\right)^2\right]$
A_{2u}	$\cos\pi\frac{2k+1}{2}x\sin\pi\frac{2\ell+1}{2}y+(-1)^{k+\ell}\cos\pi\frac{2\ell+1}{2}x\sin\pi\frac{2k+1}{2}y$ $E=\frac{\pi^2}{2}\left[\left(\frac{2k+1}{2}\right)^2+\left(\frac{2\ell+1}{2}\right)^2\right]$

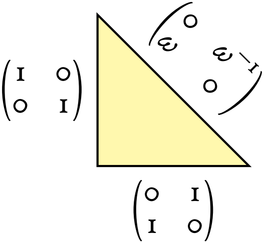
Boundary conditions

The more powerful lemma will be needed here. Here's how the two 2-dimensional representations behave ($\omega = \mathrm{e}^{2\pi\mathrm{i}/3}$):



Boundary conditions for E_g

- **Left side:** $\lambda = 1$, any vector is an eigenvector
- **Bottom side:** $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ with $\lambda = 1$;
  $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ with $\lambda = -1$.
- **Diagonal:** $\begin{pmatrix} \mathbf{e}^{-i\pi/3} \\ \mathbf{e}^{i\pi/3} \end{pmatrix}$ with $\lambda = 1$;
  $\begin{pmatrix} \mathbf{e}^{-i\pi/3} \\ -\mathbf{e}^{i\pi/3} \end{pmatrix}$ with $\lambda = -1$.



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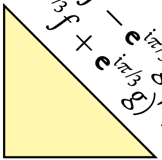
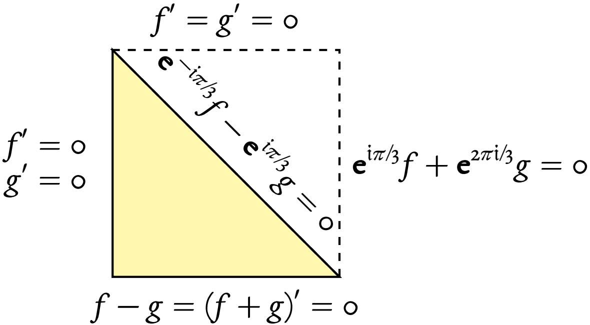


Boundary conditions for E_g

Let's add a second triangle to make a square:



Boundary conditions for E_g

Let's add a second triangle to make a square:

$f' = g' = 0$

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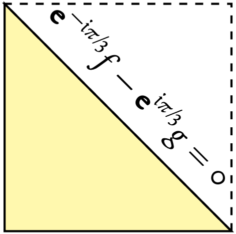

$\mathrm{e}^{\mathrm{i}\pi/3} f + \mathrm{e}^{2\pi\mathrm{i}/3} g = 0$

$f - g = (f + g)' = 0$

Set: $f - g = \varphi, \quad \mathrm{e}^{\mathrm{i}\pi/3} f + \mathrm{e}^{2\pi\mathrm{i}/3} g = \chi.$

Boundary conditions for E_g

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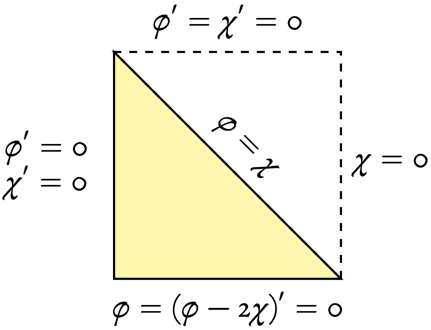


Set: $f - g = \varphi, \quad \mathrm{e}^{\mathrm{i}\pi/3} f + \mathrm{e}^{2\pi\mathrm{i}/3} g = \chi.$

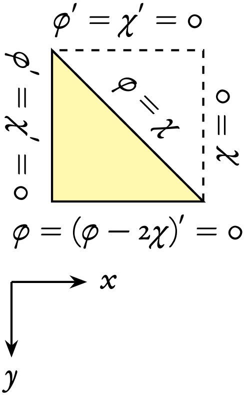
Solutions for E_g

Now we have a reasonable set of boundary conditions for those φ, χ. We may solve for them. In general, we obtain

$$\varphi = \sum_{k=0}^{\infty} c_k \cos \pi \frac{2k+1}{2} x \cos \sqrt{2E - \left(\frac{2k+1}{2}\pi\right)^2}\, y,$$

$$\chi = \sum_{k=0}^{\infty} d_k \cos \pi \frac{2k+1}{2} y \cos \sqrt{2E - \left(\frac{2k+1}{2}\pi\right)^2}\, x,$$

with $\varphi = \chi$ on the diagonal and $(\varphi - 2\chi)' = 0$ on the bottom.



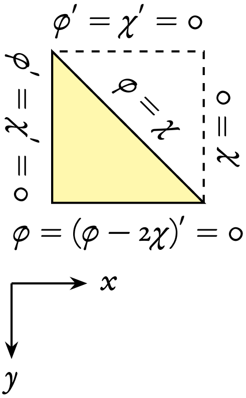
Solutions for E_g

In fact, from the matrix for the diagonal flip we can infer that $\varphi(x, y) = \chi(y, x)$. So in the end, we need to solve

$$\varphi = \sum_{k=0}^{\infty} c_k \cos \pi \frac{2k+1}{2} x \cos \sqrt{2E - \left(\frac{2k+1}{2}\pi\right)^2}\, y,$$

$$\chi = \sum_{k=0}^{\infty} c_k \cos \pi \frac{2k+1}{2} y \cos \sqrt{2E - \left(\frac{2k+1}{2}\pi\right)^2}\, x,$$

with $(\varphi - 2\chi)' = 0$ on the bottom.



Numerical solution

This can be – at least formally – solved by expanding $\left.\frac{\partial(\varphi-2\chi)}{\partial y}\right|_{y=1}$ into Fourier series. That gives a "$\infty \times \infty$" homogeneous linear system $\mathcal{F}(E)_\ell^k c_k = 0$. So c_k's can be obtained as the kernel of $\mathcal{F}(E)$ (which is mostly zero).

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As a proof of concept, we "just" feed this into the computer to obtain the energies and the c_k's by truncating the system.

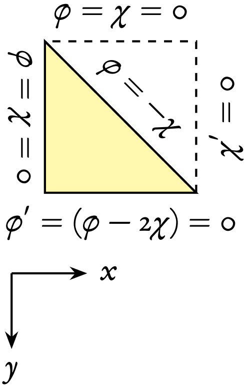
Solutions for E_u

Now the process can be repeated, just with different matrices. Now we get

$$\varphi = \sum_{k=0}^{\infty} c_k \sin \pi \frac{2k+1}{2} x \sin \sqrt{2E - \left(\frac{2k+1}{2}\pi\right)^2}\, y,$$

$$\chi = -\sum_{k=0}^{\infty} c_k \sin \pi \frac{2k+1}{2} y \sin \sqrt{2E - \left(\frac{2k+1}{2}\pi\right)^2}\, x,$$

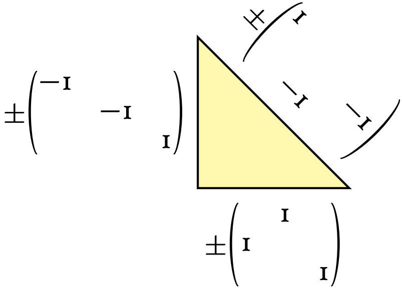
with $\varphi - 2\chi = 0$ on the bottom.

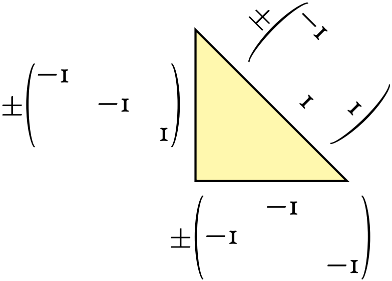


Boundary conditions

Now we just turn the crank and get more and more solutions.
Call the basis functions f, g, h.

$T_{1\mathrm{u}}^{\mathrm{g}}$	$T_{2\mathrm{u}}^{\mathrm{g}}$





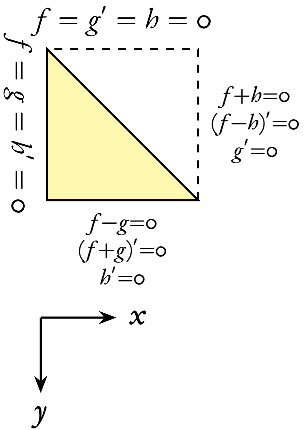
Solutions for T_{1g}

If we flip along the diagonal, we have $f \to f, g \to -h, h \to -g$. Hence,

$$f = \sum_{k=0}^{\infty} c_k \left[\sin \pi \frac{2k+1}{2} x \sin \sqrt{2E - \left(\frac{2k+1}{2}\pi\right)^2} y + \sin \pi \frac{2k+1}{2} y \sin \sqrt{2E - \left(\frac{2k+1}{2}\pi\right)^2} x \right],$$

$$g = \sum_{k=0}^{\infty} d_k \sin \pi \frac{2k+1}{2} x \cos \sqrt{2E - \left(\frac{2k+1}{2}\pi\right)^2} y,$$

$f - g = (f+g)' = 0$ on the bottom; $h(x,y) = -g(y,x)$.



Solutions for T_{1g}, cont.

Here we have two sequences of coefficients that we need to determine (both c_k and d_k). However, there are two conditions for them: $f - g = 0$ and $(f + g)' = 0$ (both at $y = 1$). So we can just use the same dumb procedure of finding the solutions using a computer.

Solutions for T_{1u}

The same method works for T_{1u}...

$$f = \sum_{k=0}^{\infty} c_k \left[\cos \pi \frac{2k+1}{2} x \cos \sqrt{2E - \left(\frac{2k+1}{2} \pi \right)^2} y - \right.$$

$$\left. - \cos \pi \frac{2k+1}{2} y \cos \sqrt{2E - \left(\frac{2k+1}{2} \pi \right)^2} x \right],$$

$$g = \sum_{k=0}^{\infty} d_k \cos \pi \frac{2k+1}{2} x \sin \sqrt{2E - \left(\frac{2k+1}{2} \pi \right)^2} y,$$

with $f + g = (f - g)' = 0$ on the bottom and $h(x, y) = g(y, x)$.

Solutions for T_{2g}

... and for T_{2g}...

$$f = \sum_{k=0}^{\infty} c_k \left[\sin \pi k x \sin \sqrt{2E - \pi^2 k^2}\, y - \sin \pi k y \sin \sqrt{2E - \pi^2 k^2}\, x\right],$$

$$g = \sum_{k=0}^{\infty} d_k \sin \pi k x \cos \sqrt{2E - \pi^2 k^2}\, y,$$

with $f + g = (f - g)' = 0$ on the bottom and $h(x, y) = g(y, x)$.

Solutions for T_{2u}

... and for T_{2u} too.

$$f = \sum_{k=0}^{\infty} c_k \left[\cos \pi kx \cos \sqrt{2E - \pi^2 k^2}\, y + \cos \pi ky \cos \sqrt{2E - \pi^2 k^2}\, x\right],$$

$$g = \sum_{k=0}^{\infty} d_k \cos \pi kx \sin \sqrt{2E - \pi^2 k^2}\, y,$$

with $f - g = (f + g)' = 0$ on the bottom and $h(x, y) = -g(y, x)$.

How to check the solutions

Now we need to check that all the solutions we obtained actually solve the equation on the whole cube.

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On the faces and the edges, the check is trivial because it's essentially flat.

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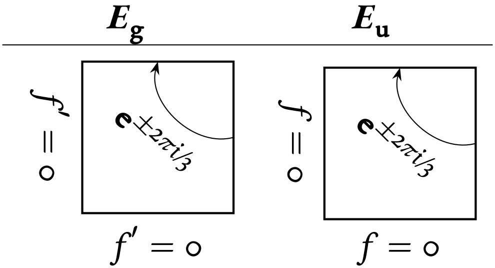
To check it at the vertices, we use the following fact: in a 2-D plane, the Laplacian can be found from the average of a function taken over a little sphere like this:

$$\oint_{|x-x_0|=r} f(x)\,\mathrm{d}x = f(x_0) + \tfrac{1}{4}(\Delta f)(x_0)r^2 + o(r^2) \quad \text{as } r \to 0.$$

If we take this as a *definition* of the Laplacian, we can extend it to the vertices easily, and check that our solutions satisfy the Helmholtz equation.

Equivalent problems

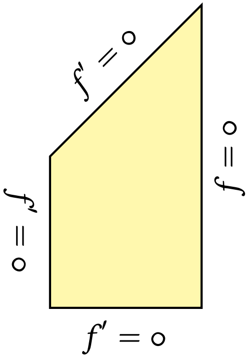
Solving the double-degenerate case is equivalent to solving the Helmholtz equation on a square like this:



Here, the arrow means that one of the sides must be $e^{\pm 2\pi i/3}$ times the other, and the normal derivative must be $-e^{\pm 2\pi i/3}$ times the other.

Equivalent problems

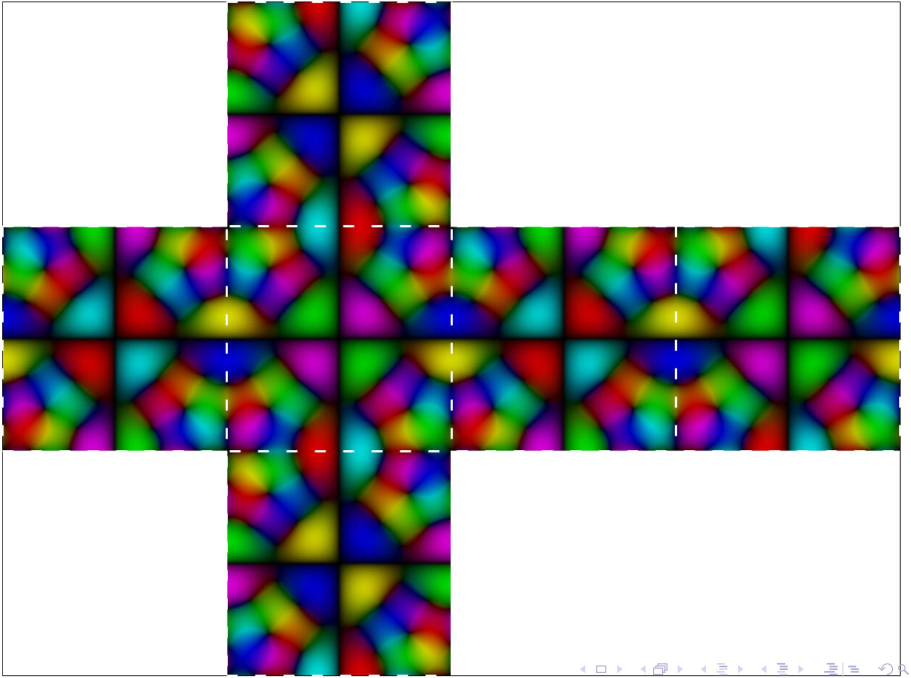
Solving the triple-degenerate case is equivalent to solving the Helmholtz equation on a weird quadrangle, for instance



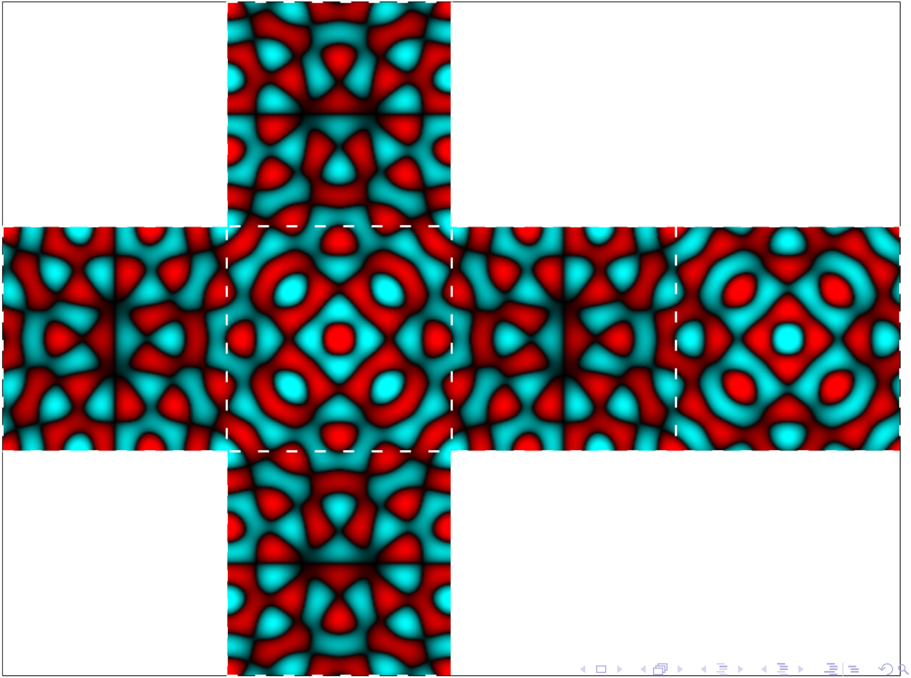
Equivalent problems

I don't think any of these have been solved yet.

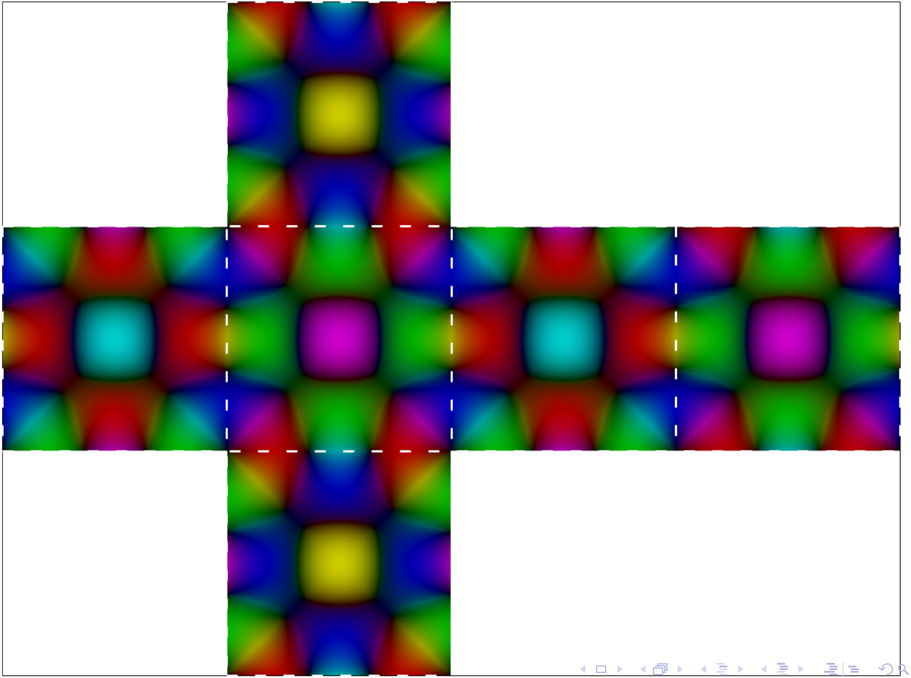
E_u mode no. 5, E = 46.15341375340444



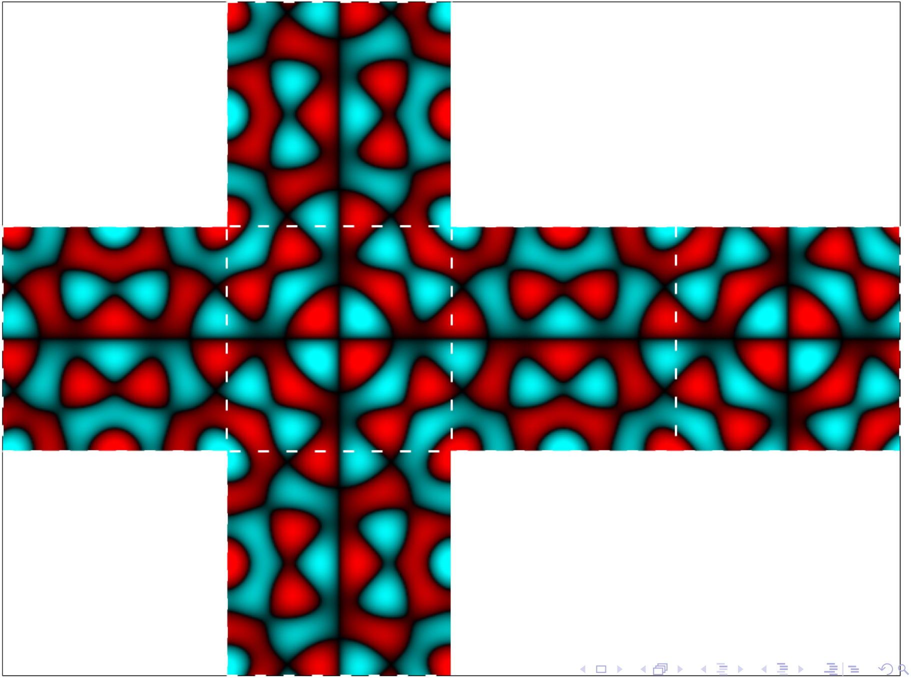
T_{2u} mode no. 35, E = 132.2141



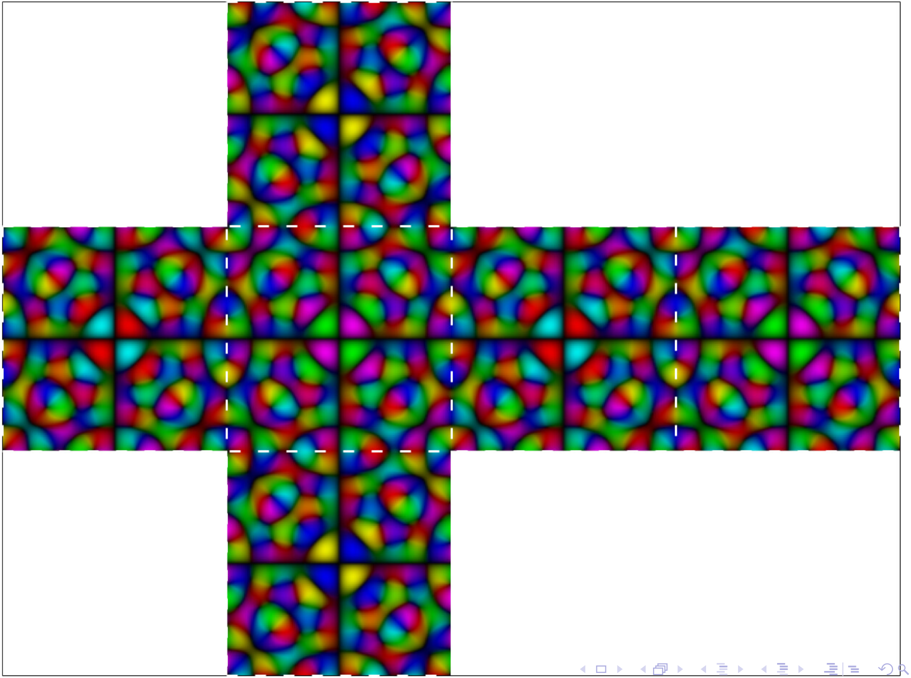
E_g mode no. 3, E = 17.85080495122557



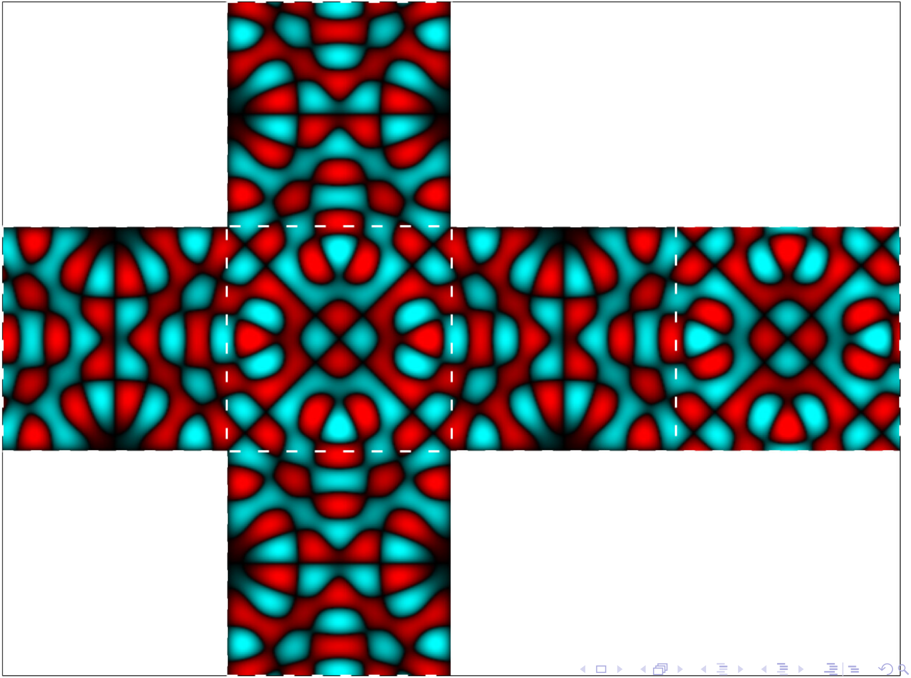
T_{1g} mode no. 15, E = 64.3266



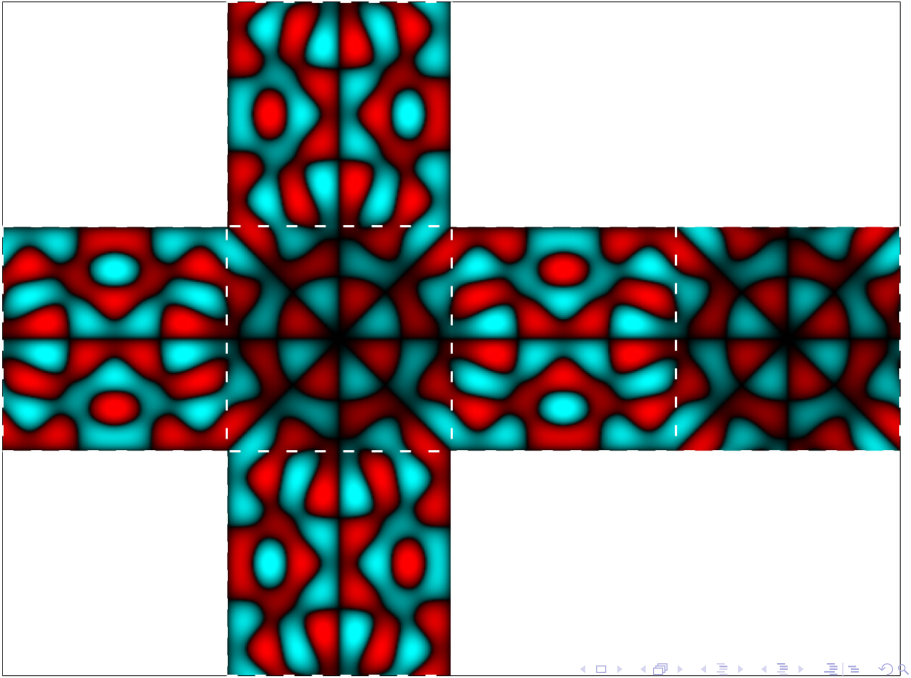
E_u mode no. 22, E = 156.885266566476I



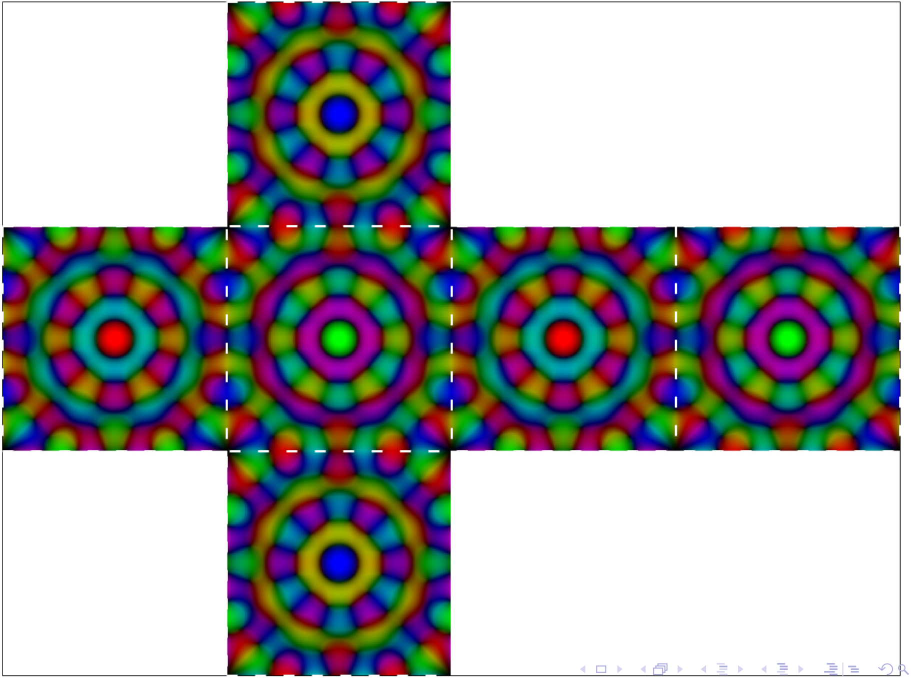
T_{1u} mode no. 27, E = 121.5351



T_{2g} mode no. 17, E = 89.1242



E_g mode no. 18, E = 103.6506445610297



Thank you!