

# Quantum graphs illustrated

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ABSTRACT. This is an introduction to the quantum graphs, and their potential applications to physics. We use a simple formalism for such graphs, with these coming from a vertex set  $X$ , which is a quantum space, dual to a finite dimensional  $C^*$ -algebra  $A = C(X)$ , and an adjacency matrix over this vertex set,  $d \in \mathcal{L}(A) \simeq M_N(\mathbb{C})$  with  $N = |X| = \dim A$ , that we will often assume self-adjoint,  $d = d^*$ . Intuitively, the “points” of  $X$  can be thought of as being the indices  $(i, j, k)$  of the standard multimatrix basis  $\{e_{ij}^k\}$  of the algebra  $A$ , and the entries of  $d$  can be thought of as being colored arrows between these points, and we will base our study on this observation.

## Preface

What is a quantum graph? Good question, with the answer to this depending on how much complicated you want to be, and what potential applications you have in mind. In short, many choices here, depending on your mathematical philosophy.

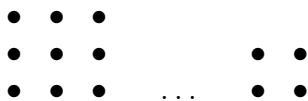
In this book we will go for the simplest axioms, with the idea in mind that “simple mathematics should correspond to true physics”. This is of course something subjective, but I’m saying this as a mathematical physicist, surrounded by both mathematicians and physicists, on a daily basis. The only point of agreement between everyone are theories involving simple mathematics. And everything else is poised to be hotly debated for some time, with even insults of type “wrong” being formulated, and eventually forgotten.

But probably too much talking, let us axiomatize the quantum graphs. We need vertices and edges for them, and our story here will be as follows:

(1) First we need a vertex set, which must be a “finite quantum space”. According to von Neumann, the quantum spaces are the duals of operator algebras, and when adopting this viewpoint, problem solved, because what we need is a finite dimensional  $C^*$ -algebra  $A$ , and then we can formally write  $A = C(X)$ , and we have our vertex set  $X$ .

(2) You might perhaps ask at this point, but what are the points of  $X$ ? Very natural question, with versions and duplicates of this regularly flooding the internet. So, in answer, let me ask you a question too, are you here for quantum, or not? In quantum we have no points, and not only this is not a problem, but we are proud of this.

(3) This being said, something can be done here. Since our algebra  $A$  must be a direct sum of matrix algebras,  $A = M_{n_1}(\mathbb{C}) \oplus \dots \oplus M_{n_k}(\mathbb{C})$ , we can represent each matrix block as a square, and we end up with a picture like this, representing  $A$ :

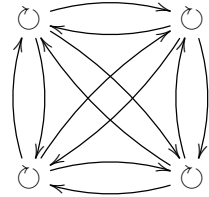


(4) But looking at this picture, we can say that this represents  $X$  itself. For instance the number of points is the correct one,  $|X| = \dim A$ . Also, in the case  $A = \mathbb{C}^N$ , the

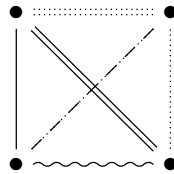
picture that we get,  $\bullet \bullet \dots \bullet$ , is the correct picture of  $X$ , as a space of points. More generally, when  $n_i = 1$ , the associated point  $\bullet$  is a true point of  $X$ . And so on.

(5) With this done, let us turn now to edges. Here we need an adjacency matrix over the vertex set,  $d \in \mathcal{L}(A) \simeq M_N(\mathbb{C})$ , with  $N = |X| = \dim A$ . Thus, good news, no need for complicated mathematics here, what we need is a usual matrix  $d \in M_N(\mathbb{C})$ .

(6) As further good news, we can represent  $d \in M_N(\mathbb{C})$  on our picture of  $X$ , by drawing an arrow  $i \rightarrow j$  between any two points, and coloring it with the complex number  $d_{ij} \in \mathbb{C}$ . As an example here, in the case  $A = M_2(\mathbb{C})$  we end up with a picture as follows, with all arrows being supposed to be colored, but with the colors missing, due to budget cuts:



(7) Of course, we can impose some natural conditions on  $d$ . For instance when assuming that  $d$  is symmetric, and has 0 on the diagonal, as the usual adjacency matrices of graphs do, the generic picture looks as follows, this time without budget cuts:



So done, so we have now our definition of quantum graphs, along with pictures for them, which are very similar to the usual graphs, and can help us with our math.

We will talk about such beasts in this book, focusing on their algebraic, geometric and analytic aspects, and their potential applications to physics. The theory will be quite elementary, to start with, usual linear algebra and graph theory, regarded from a different perspective, as you can see from the above. However, when looking at the “quantum symmetries” of such beasts, and potential applications to physics, we will soon run into infinite dimensions, and other subtle phenomena. So, do not worry, we will have some non-trivial mathematics too, but kept of course as simple as possible.

Many thanks go to my colleagues, for joint work and discussions on quantum graphs, quantum groups, and related topics. Thanks as well to my cats. They say that mice use only classical graphs, for their orientation, and that this is a slight weakness.

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Part I

Quantum graphs

*Don't say it in Russian*  
*Don't say it in German*  
*Say it in broken English*  
*Say it in broken English*

## CHAPTER 1

### Quantum spaces

#### 1a. Linear algebra

Welcome to physics. Or almost. We will be doing mostly mathematics in this book, strongly motivated however by quantum mechanics, and statistical mechanics. As a first trick that I want to teach you, whenever into a new math theory, check the following:

- (1) Are there matrices and operators everywhere?
- (2) What about groups and probability, are these involved too?
- (3) Does the theory claim zero applications to classical problems?
- (4) Is the theory simple enough, or at least advertised as such?

If these conditions are satisfied, you can be pretty much sure that the theory in question is about quantum and statistical mechanics. So, if you love these two disciplines of physics, which are both beautiful, and fascinating, go ahead and learn that theory.

If not, you are of course welcome to stay, but bear in mind that you might have at some point to face (3), with “classical problems” there meaning classical mechanics, fluid mechanics, basic thermodynamics, electrostatics, magnetostatics and basic electrodynamics, including electric machinery like the usual computers, and so finally everything science and engineering, and related mathematics, which is somewhat “old-style”. Needless to say, all this old-style science and mathematics can be very complicated, and if you love that, this is very good, we all love that mathematics and physics, and there are plenty of exciting problems there, waiting for you. But, just of matter of not mixing up things, if (3) is there, that might be a source of troubles later, don’t overestimate yourself.

Finally, in case you are a pure mathematician, I would say have a look at what you’re doing, the story of your math subject I mean, and find out what sort of physics, classical or non-classical, was there at the beginning. Most likely that type of physics is still there, now as we talk, perhaps in some hidden form, and so will it be in the foreseeable future, better count on that. So, that would be the least of things, figure out all this, which will give you some intuition on your math objects, and most likely boost the quality of your research by 10. And then, in regards to what is to be learned, act accordingly.

Getting to the present book, you guessed right, our aim here will be to explain a certain mathematical theory, fulfilling (1-2-3-4), and so most likely, potentially useful in quantum and statistical mechanics. We will build our theory on standard mathematics as that comes, meaning Rudin [78], with some algebra knowledge, say from Lang [61], being welcome too. As for the physics, we will sort of assume that you are a bit familiar with the basics, say learned from the undergraduate course of Feynman [34].

What shall we start with? Matrices, of course, as per our requirement (1). So, here is a crash course in basic linear algebra, and you surely know all this:

THEOREM 1.1. *The following happen:*

- (1) *The linear maps  $f : \mathbb{R}^N \rightarrow \mathbb{R}^N$  are precisely the maps of the form  $f(x) = Ax$ , with  $x$  being written as column vector, and with  $A \in M_N(\mathbb{R})$ .*
- (2) *When  $A$  is diagonalizable, with eigenvalues  $\lambda_i$  and eigenvectors  $v_i$ , the map  $f$  can be understood geometrically, as multiplying by  $\lambda_i$  in each direction  $v_i$ .*
- (3) *The matrices  $A \in M_N(\mathbb{R})$  are generically not diagonalizable, but when regarded as complex matrices,  $A \in M_N(\mathbb{C})$ , they become generically diagonalizable.*
- (4) *Thus, it is better to look at the linear maps  $f : \mathbb{C}^N \rightarrow \mathbb{C}^N$ , which are the maps of the form  $f(x) = Ax$ , with  $x$  column vector, and  $A \in M_N(\mathbb{C})$ .*

PROOF. All this is standard linear algebra, the idea being as follows:

(1) This is clear, because  $f$  being linear means that  $f(x) = y$  varies linearly with  $x$ , and so that  $y_i = \sum_j A_{ij}x_j$ , for some  $A_{ij} \in \mathbb{R}$ . Thus, we have our matrix.

(2) This is actually the definition of the diagonalization, and if you see here a theorem instead of a definition, you probably got it wrong, with your linear algebra.

(3) This is something subtle, with the first assertion coming from the fact that the probability for the roots  $\lambda \in \mathbb{C}$  of the characteristic polynomial  $P_A$  to be real is obviously  $P = 0$ . As for the second assertion, this comes from the fact that any matrix with distinct eigenvalues is diagonalizable, because the probability for our matrix to lie on the hypersurface  $\Delta(P_A) = 0$ , with  $\Delta$  being the discriminant, is clearly  $P = 0$ .

(4) This is a conclusion coming from (3), which tells us to say goodbye to  $\mathbb{R}$ , unless having some good reasons to be attached to it, and we haven't any, at this point, and work with  $\mathbb{C}$  instead. Of course, this is a bit subjective, and in addition making our Theorem a dynamic object, with (4) replacing (1). More physics here, than math, I guess.  $\square$

At a more advanced level now, the idea is that we can do some geometry, for our linear maps and matrices, by using the scalar product on  $\mathbb{C}^N$ , given by:

$$\langle x, y \rangle = \sum_i x_i \bar{y}_i$$

To be more precise, we have the following result, in relation with the scalar products, and what can be done with them, that you surely know too:

**THEOREM 1.2.** *The following happen:*

- (1) *Each linear map  $f : \mathbb{C}^N \rightarrow \mathbb{C}^N$  has an adjoint map  $f^* : \mathbb{C}^N \rightarrow \mathbb{C}^N$ , given by the formula  $\langle f(x), y \rangle = \langle x, f^*(y) \rangle$ , for any  $x, y \in \mathbb{C}^N$ .*
- (2) *At the matrix level, assuming  $f(x) = Ax$ , we have  $f^*(x) = A^*x$ , with  $A^* \in M_N(\mathbb{C})$  being the adjoint matrix, given by  $(A^*)_{ij} = \bar{A}_{ji}$ .*
- (3) *The orthogonal projections are given by matrices satisfying  $P = P^* = P^2$ , and the isometries, or unitaries, are given by matrices satisfying  $U^* = U^{-1}$ .*
- (4) *Any matrix which is self-adjoint,  $A = A^*$ , or more generally normal,  $AA^* = A^*A$ , is diagonalizable, with the passage matrix being unitary.*

**PROOF.** All this is again standard linear algebra, the idea being as follows:

(1) This is clear, because given  $y \in \mathbb{C}^N$ , the map  $\varphi(x) = \langle f(x), y \rangle$  is linear, and so we must have  $\varphi(x) = \langle x, z \rangle$ , for some  $z \in \mathbb{C}^N$ , that we can call  $z = f^*(y)$ .

(2) This comes from the formula in (1) via the fact that, for a linear map  $f(x) = Ax$ , the matrix  $A$  can be recaptured via the formula  $A_{ij} = \langle f(e_j), e_i \rangle$ .

(3) The first assertion is standard, with the condition  $P = P^2$  guaranteeing for an oblique projection, and with  $P = P^*$  needing to be added, as for this projection to be orthogonal. As for the second assertion, the point here is that  $\|Ux\| = \|x\|$  is equivalent, via the polarization identity, to  $\langle Ux, Uy \rangle = \langle x, y \rangle$ , which reads  $U^* = U^{-1}$ .

(4) This is something heavier, called spectral theorem. For the self-adjoints,  $A = A^*$ , the result is quite easy to obtain, with the first step being that of proving that the eigenvalues are real,  $\lambda \in \mathbb{R}$ . Then we have a version of this result for the unitaries,  $A^* = A^{-1}$ , where the eigenvalues are on the unit circle,  $\lambda \in \mathbb{T}$ . And finally, the general normal case,  $AA^* = A^*A$ , uses a mixture of self-adjoint and unitary techniques.  $\square$

All this is very beautiful mathematics, having countless applications, and to end this crash course in linear algebra, a question that I have for you:

**QUESTION 1.3.** *How does the rotation of angle  $t$  in the plane, namely*

$$R_t = \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix}$$

*diagonalize, in view of the fact that it has no obvious eigenvectors?*

As a joke here, personally it took me about 10-15 years of work, both teaching and research, in order to fully digest the answer to this question. The thing being that, when I was younger, I was often waking up at night, saying to myself that all the linear algebra I know is wrong. But gone all this, no longer such nightmares, now that I got older.

Back to our business now, we have the following question:

QUESTION 1.4. *Where is the quantum physics, in relation with all this?*

We will attempt to answer here this question, first with some cheap mathematical speculations, and then with some serious physics from 100 years ago, following Lyman, Balmer, Paschen, then Ritz-Rydberg, and finally Heisenberg, and Schrödinger, and Dirac too. And once we will get convinced that there is quantum physics behind all this, we will take matters seriously, talk matrices and operators following von Neumann, and eventually, switching back to finite dimensions, get to quantum graphs.

So, let us start with some mathematical speculations. We first have:

SPECULATION 1.5. *Since the algebra  $A = M_2(\mathbb{C})$  is isomorphic as vector space with  $\mathbb{C}^4 = C(1, 2, 3, 4)$ , we can think of it as being of the following form, with  $M_2$  being some sort of “quantum space”, and with  $\sim$  standing for some sort of “twisting”:*

$$A = C(M_2) \quad , \quad M_2 \sim \{1, 2, 3, 4\}$$

*And this quantum space  $M_2$  might be useful in dealing with quantum mechanics, where things are a bit “fuzzy”, with the particles having undefined positions and speeds.*

And take this as this comes, with this depending on your physics knowledge. To be more precise, you surely know that in quantum mechanics things are a bit “fuzzy”, as said above, and so anything mathematical of classical type, be that usual curves, surfaces, manifolds  $X \subset \mathbb{R}^N$ , or even finite spaces like  $\{1, 2, 3, 4\}$ , which were originally designed in order to help with classical mechanics, will normally fail in that setting. Thus, we are genuinely interested in all sorts of crazy mathematical “quantum spaces”, any idea being welcome, in the hope that such spaces can help us in quantum mechanics.

In a word, Speculation 1.5, and anything similar, is definitely welcome. But then, thinking a bit more at all this, the above space  $M_2$  is not that crazy as it seems, I mean come up if you can with a mathematical construction of a “quantum space” which is less crazy. So, as a conclusion, Speculation 1.5 is not only welcome, but warmly welcome, if the gods of quantum mechanics are with us, spaces like  $M_2$  might be the answer.

Less speculatively now, and assuming that you know some physics, you surely know that talking about the electron spin requires the Pauli matrices, which form a basis of the algebra  $M_2(\mathbb{C})$ . Thus, Speculation 1.5 is in fact something corresponding to a deep finding in physics, and worth a Nobel Prize, that won by Pauli for his work.

In any case, beginner level or not, you must agree with me that Speculation 1.5 is something to be taken seriously. So, let us further speculate on that. We have:

SPECULATION 1.6. *Regarding  $M_2$ , we can even have a geometric picture of it,*

$$\begin{array}{cc} \bullet_{11} & \bullet_{12} \\ \bullet_{21} & \bullet_{22} \end{array}$$

*with each formal point  $\bullet_{ij}$  standing for the corresponding elementary matrix*

$$e_{ij} : e_j \rightarrow e_i$$

*based on the observation that these matrices form a basis of  $A = C(M_2)$ .*

To be more precise here, let us first examine the classical space  $X = \{1, 2, 3, 4\}$ . We can represent this space by a series of 4 points, as everyone does, as follows:

$$\bullet_1 \quad \bullet_2 \quad \bullet_3 \quad \bullet_4$$

Now if we look at the algebra of functions  $C(X) = \mathbb{C}^4$ , this is spanned by the Dirac masses  $\delta_i$ , one for each of the points  $\bullet_i$ . Thus, we can say that “spaces are described by the functions on them”, and we are led in this way to the above picture of  $M_2$ .

All this is quite interesting, we have some beginning of mathematics here, for our mysterious space  $M_2$ . And we can further speculate on this, in the following way:

SPECULATION 1.7. *The twisting operation  $\{1, 2, 3, 4\} \rightarrow M_2$ , which reads*

$$\begin{array}{ccccccc} & & & & & \bullet_{11} & \bullet_{12} \\ & & & & & & \\ \bullet_1 & \bullet_2 & \bullet_3 & \bullet_4 & \rightsquigarrow & & \\ & & & & & \bullet_{21} & \bullet_{22} \end{array}$$

*amounts in changing the multiplication rule on the vector space  $\mathbb{C}^4$ , as follows,*

$$e_i e_j = \delta_{ij} e_i \quad \rightsquigarrow \quad e_{ij} e_{kl} = \delta_{jk} e_{il}$$

*at the level of the standard basis, in each case.*

To be more precise, here we are using the same philosophy as for Speculation 1.6, namely that “spaces are described by the functions on them”, and in what regards the multiplication formulae, we first have  $e_i e_j = \delta_{ij} e_i$ , which is the familiar multiplication rule for the Dirac masses on  $\{1, 2, 3, 4\}$ , and then we have  $e_{ij} e_{kl} = \delta_{jk} e_{il}$ , which is the familiar multiplication rule for the matrix units  $e_{ij} : e_j \rightarrow e_i$ , from Speculation 1.6.

As a further comment here, coming as a continuation of our previous comment on the Pauli matrices, in case you are familiar with these, you might argue that why using  $e_{ij}$  instead of these Pauli matrices. Good point, and we will be back to this, later.

As another speculation now, using adjoint matrices and positivity, we have:

SPECULATION 1.8. *We can compute expectations over  $M_2$ , according to*

$$\mathbb{E}(f) = \frac{f_{11} + f_{22}}{2}$$

*with the basic requirements  $\mathbb{E}(1) = 1$ , and  $f \geq 0 \implies \mathbb{E}(f) \geq 0$ , being satisfied.*

To be more precise, we are using here the same philosophy as before, with the functions  $f \in C(M_2)$  being by definition the matrices  $f \in M_2(\mathbb{C})$ . Now if we consider the trace of matrices, normalized as above, as to have  $\text{tr}(1) = 1$ , we have  $\text{tr}(gg^*) \geq 0$  for any  $g$ , which via a bit more linear algebra means  $f \geq 0 \implies \text{tr}(f) \geq 0$ . Thus, this normalized trace satisfies what we can expect from an expectation, and we can set  $\mathbb{E} = \text{tr}$ .

It is possible to speculate some more, along the same lines, but enough work done for the day, let us formulate our conclusions, which are quite good, as follows:

CONCLUSION 1.9. *Spaces like  $M_2$  are the simplest possible “quantum spaces”, mathematically speaking, and we definitely have tools, including pictures, for dealing with them. With a bit of luck, these might help in quantum physics, which needs such spaces.*

Of course, all this was a bit subjective, and many things remain to be clarified. But no worries, we will be back to this soon, with full mathematical details.

### 1b. Quantum physics

Very nice the above, but thinking a bit, the physics input in all that was quite slim, basically amounting in you and me agreeing on the fact that things are quite “fuzzy” in quantum physics, with the particles there having no clear positions and speeds, and therefore with quantum physics being most likely in need of beasts such as  $M_2$ .

Of course we made some comments too in relation with the Pauli matrices, which are more advanced, but the truth is, what we did so far was mostly mathematics, with minimal physics input. So, time now to get into more physics, in order to answer:

QUESTION 1.10. *Leaving aside the above speculations, which are nice but mostly mathematical, are matrices really needed in quantum physics?*

Which leads us into the preliminary question, what is actually quantum physics. Not an easy question, and believe me, people like Maxwell, or Lorentz, or Planck, or Einstein, or Balmer, or Rydberg, or Bohr, or Becquerel, or Pierre and Marie Curie, who all knew what they were doing, would have loved to have an answer to this, around 1900.

In answer, retrospectively, quantum physics is the fix for electrodynamics, and for the Maxwell equations. And with these Maxwell equations working perfectly at the macroscopic level, but failing at the level of the simplest microscopic problem, that of an elementary negative charge spinning around an elementary positive charge, that is, failing to understand the functioning of the hydrogen atom, we can formulate, as definition:



DEFINITION 1.11. *Quantum physics is the understanding of the hydrogen atom, and of related physics questions, at about the same scale,  $1 \text{ nm} = 10^{-9} \text{ m}$  and below.*

So, hydrogen atom, that is the starting point for everything. But how to investigate it? You would say, put it under a good microscope, but believe me, that will not work, because even nowadays, the best microscope technology has a very bad resolution, with respect to the size of the hydrogen atom. Plus, who knows, even when assuming our problem solved, and centering our microscope on the proton, the electron might be too fast to move for us to see, or be “slippery”, in all sorts of other weird ways.

Fortunately, the answer to this question is very simple, coming from spectroscopy. Simply burn, or rather heat, hydrogen, and record the color of the spectral lines that you get, that data is simply to get, and is golden. In order to discuss this, we will need the following standard fact, coming from the mathematics of the Maxwell equations:

FACT 1.12. *An accelerating or decelerating charge produces electromagnetic waves, travelling in vacuum at speed  $c = 299,792,458$ , following the wave equation*

$$\ddot{\varphi} = c^2 \Delta \varphi$$

*and in non-vacuum at a lower speed  $v < c$ , following  $\ddot{\varphi} = v^2 \Delta \varphi$ . These waves are called light, whose frequency and wavelength can be explicitly computed.*

To be more precise, this phenomenon can be observed in a variety of situations, such as the usual light bulbs, where electrons get decelerated by the filament, acting as a resistor, or in usual fire, which is a chemical reaction, with the electrons moving around, as they do in any chemical reaction, or in machinery like nuclear plants, particle accelerators, and so on, leading there to all sorts of eerie glows, of various colors. As mentioned above, the explanation for this comes from the mathematics of the Maxwell equations.

Moving ahead with optics, we will need here the following standard fact:

FACT 1.13. *When travelling through a material, and hitting a new material, some of the light gets reflected, at the same angle, and some of it gets refracted, at a different angle, depending both on the old and the new material, and on the wavelength.*

There are many things that can be said here. As a basic formula, we have the famous Snell law, which relates the incidence angle  $\theta_1$  to the refraction angle  $\theta_2$ , as follows:

$$\frac{\sin \theta_2}{\sin \theta_1} = \frac{n_1(\lambda)}{n_2(\lambda)}$$

Here  $n_i(\lambda)$  are the refraction indices of the two materials, adjusted for the wavelength, and with this adjustment for wavelength being the whole point, which is something quite complicated. Now as a simple consequence of the above fact, we have:

FACT 1.14. *Light can be decomposed, by using a prism.*

Thus, we can study events via spectroscopy, by capturing the light the event has produced, decomposing it with a prism, recording its “spectral signature”, consisting of the wavelenghts present, and their density, and then doing some reverse engineering.

Back to hydrogen, first on our list is the following discovery, by Lyman in 1906:

FACT 1.15 (Lyman). *The hydrogen atom has spectral lines given by the formula*

$$\frac{1}{\lambda} = R \left( 1 - \frac{1}{n^2} \right)$$

where  $R \simeq 1.097 \times 10^7$  and  $n \geq 2$ , which are as follows,

$n$	Name	Wavelength	Color
—	—	—	—
2	$\alpha$	121.567	UV
3	$\beta$	102.572	UV
4	$\gamma$	97.254	UV
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\infty$	limit	91.175	UV

called *Lyman series of the hydrogen atom*.

Observe that all the Lyman series lies in UV, which is invisible to the naked eye. Due to this fact, this series, while theoretically being the most important, was discovered only second. The first discovery, which was the big one, and the breakthrough, was by Balmer, the founding father of all this, back in 1885, in the visible range, as follows:

FACT 1.16 (Balmer). *The hydrogen atom has spectral lines given by the formula*

$$\frac{1}{\lambda} = R \left( \frac{1}{4} - \frac{1}{n^2} \right)$$

where  $R \simeq 1.097 \times 10^7$  and  $n \geq 3$ , which are as follows,

$n$	Name	Wavelength	Color
—	—	—	—
3	$\alpha$	656.279	red
4	$\beta$	486.135	aqua
5	$\gamma$	434.047	blue
6	$\delta$	410.173	violet
7	$\varepsilon$	397.007	UV
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\infty$	limit	346.600	UV

called *Balmer series of the hydrogen atom*.

So, this was Balmer's original result, which started everything. As a third main result now, this time in IR, due to Paschen in 1908, we have:

FACT 1.17 (Paschen). *The hydrogen atom has spectral lines given by the formula*

$$\frac{1}{\lambda} = R \left( \frac{1}{9} - \frac{1}{n^2} \right)$$

where  $R \simeq 1.097 \times 10^7$  and  $n \geq 4$ , which are as follows,

$n$	Name	Wavelength	Color
	—	—	
4	$\alpha$	1875	IR
5	$\beta$	1282	IR
6	$\gamma$	1094	IR
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\infty$	limit	820.4	IR

called Paschen series of the hydrogen atom.

Observe the striking similarity between the above three results. In fact, we have here the following fundamental, grand result, due to Rydberg in 1888, based on the Balmer series, and with later contributions by Ritz in 1908, using the Lyman series as well:

CONCLUSION 1.18 (Rydberg, Ritz). *The spectral lines of the hydrogen atom are given by the Rydberg formula, depending on integer parameters  $n_1 < n_2$ ,*

$$\frac{1}{\lambda_{n_1 n_2}} = R \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

with  $R$  being the Rydberg constant for hydrogen, which is as follows:

$$R \simeq 1.096\,775\,83 \times 10^7$$

These spectral lines combine according to the Ritz-Rydberg principle, as follows:

$$\frac{1}{\lambda_{n_1 n_2}} + \frac{1}{\lambda_{n_2 n_3}} = \frac{1}{\lambda_{n_1 n_3}}$$

Similar formulae hold for other atoms, with suitable fine-tunings of  $R$ .

Here the first part, the Rydberg formula, generalizes the results of Lyman, Balmer, Paschen, which appear at  $n_1 = 1, 2, 3$ , at least retrospectively. The Rydberg formula predicts further spectral lines, appearing at  $n_1 = 4, 5, 6, \dots$ , and these were discovered later, by Brackett in 1922, Pfund in 1924, Humphreys in 1953, and others afterwards,

with all these extra lines being in far IR. The simplified complete table is as follows:

$n_1$	$n_2$	Series name	Wavelength $n_2 = \infty$	Color $n_2 = \infty$
		—	—	
1	2 – $\infty$	Lyman	91.13 nm	UV
2	3 – $\infty$	Balmer	364.51 nm	UV
3	4 – $\infty$	Paschen	820.14 nm	IR
		—	—	
4	5 – $\infty$	Brackett	1458.03 nm	far IR
5	6 – $\infty$	Pfund	2278.17 nm	far IR
6	7 – $\infty$	Humphreys	3280.56 nm	far IR
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Regarding the last assertion, concerning other elements, this is something conjectured and partly verified by Ritz, and fully verified and clarified later, via many experiments, the fine-tuning of  $R$  being basically  $R \rightarrow RZ^2$ , where  $Z$  is the atomic number.

From a theoretical physics viewpoint, the main result remains the middle assertion, called Ritz-Rydberg combination principle, and the formula there, namely:

$$\frac{1}{\lambda_{n_1 n_2}} + \frac{1}{\lambda_{n_2 n_3}} = \frac{1}{\lambda_{n_1 n_3}}$$

The point indeed is that, mathematical speaking, this combination formula reminds the multiplication rule for the elementary matrices  $e_{ij} : e_j \rightarrow e_i$ , namely:

$$e_{n_1 n_2} e_{n_2 n_3} = e_{n_1 n_3}$$

All this is very interesting, and leads to the following principle, due to Heisenberg:

**PRINCIPLE 1.19 (Heisenberg).** *Observables in quantum mechanics should be some sort of infinite matrices, generalizing the Lyman, Balmer, Paschen lines of the hydrogen atom, and multiplying between them as the matrices do, as to produce further observables.*

This principle is something quite deep, and needs a number of comments, namely:

(1) First of all, our matrices must be indeed infinite, because so are the series observed by Lyman, Balmer, Paschen, corresponding to  $n_1 = 1, 2, 3$  in the Rydberg formula, and making it clear that the range of the second parameter  $n_2 > n_1$  is up to  $\infty$ .

(2) Although this was not known to Ritz-Rydberg and Heisenberg, as mentioned above, some later results of Brackett, Pfund, Humphreys and others, at  $n_1 = 4, 5, 6, \dots$ , confirmed the fact that the range of the first parameter  $n_1$  is up to  $\infty$  too.

(3) As a more tricky comment now, going beyond what Principle 1.19 says, our infinite matrices must be in fact complex. This was something known to Heisenberg, and later Schrödinger came with proof that quantum mechanics naturally lives over  $\mathbb{C}$ .

(4) Finally, all this leads us into some tricky mathematics, because the infinite matrices  $A \in M_\infty(\mathbb{C})$  do not act on the vectors  $v \in \mathbb{C}^\infty$  just like that. For instance the all-one matrix  $A_{ij} = 1$  does not act on the all-one vector  $v_i = 1$ , for obvious reasons.

Summarizing, in order to have to some mathematical theory going, out of Principle 1.19, we have to deal with infinite matrices  $A \in M_\infty(\mathbb{C})$  which are “bounded”, in a certain sense. However, before getting into this, let us hear as well the point of view of Schrödinger, which came a few years later. His idea was to forget about exact things, and try to investigate the hydrogen atom statistically, his question being as follows:

QUESTION 1.20. *In the context of the hydrogen atom, assuming that the proton is fixed, what is the probability density  $\varphi_t(x)$  of the position of the electron  $e$ , at time  $t$ ,*

$$P_t(e \in V) = \int_V \varphi_t(x) dx$$

*as function of an initial probability density  $\varphi_0(x)$ ? Also, can the corresponding equation be solved, and will this explain the functioning of the hydrogen atom, statistically?*

In order to get familiar with this question, let us first look at examples coming from classical mechanics. In the context of a particle whose position at time  $t$  is given by  $x_0 + \gamma(t)$ , the evolution of the probability density will be given by:

$$\varphi_t(x) = \varphi_0(x) + \gamma(t)$$

However, such examples are somewhat trivial, of course not in relation with the computation of  $\gamma$ , usually a difficult question, but in relation with our questions, and do not apply to the electron. The point indeed is that, in what regards the electron, we have:

FACT 1.21. *In respect with various simple interference experiments:*

- (1) *The electron is definitely not a particle in the usual sense.*
- (2) *But in most situations it behaves exactly like a wave.*
- (3) *But in other situations it behaves like a particle.*

Getting back now to the Schrödinger question, all this suggests to use, as for the waves, an amplitude function  $\psi_t(x) \in \mathbb{C}$ , related to the density  $\varphi_t(x) > 0$  by the formula  $\varphi_t(x) = |\psi_t(x)|^2$ . Not that a big deal, you would say, because the two are related by simple formulae as follows, with  $\theta_t(x)$  being an arbitrary phase function:

$$\varphi_t(x) = |\psi_t(x)|^2 \quad , \quad \psi_t(x) = e^{i\theta_t(x)} \sqrt{\varphi_t(x)}$$

However, such manipulations can be crucial, raising for instance the possibility that the amplitude function satisfies some simple equation, while the density itself, maybe not. And this is what happens indeed. Schrödinger was led in this way to:

CLAIM 1.22 (Schrödinger). *In the context of the hydrogen atom, the amplitude function of the electron  $\psi = \psi_t(x)$  is subject to the Schrödinger equation*

$$ih\dot{\psi} = -\frac{\hbar^2}{2m}\Delta\psi + V\psi$$

*$m$  being the mass,  $\hbar = h_0/2\pi$  the reduced Planck constant, and  $V$  the Coulomb potential of the proton. The same holds for movements of the electron under any potential  $V$ .*

Observe the similarity with the wave equation  $\ddot{\varphi} = v^2\Delta\varphi$ , and with the heat equation  $\dot{\varphi} = \alpha\Delta\varphi$  too. Many things can be said here. Following now Heisenberg and Schrödinger, and then especially Dirac, who did the axiomatization work, we have:

DEFINITION 1.23. *In quantum mechanics the states of the system are vectors of a Hilbert space  $H$ , and the observables of the system are linear operators*

$$T : H \rightarrow H$$

*which can be densely defined, and are taken self-adjoint,  $T = T^*$ . The average value of such an observable  $T$ , evaluated on a state  $\xi \in H$ , is given by:*

$$\langle T \rangle = \langle T\xi, \xi \rangle$$

*In the context of the Schrödinger mechanics of the hydrogen atom, the Hilbert space is the space  $H = L^2(\mathbb{R}^3)$  where the wave function  $\psi$  lives, and we have*

$$\langle T \rangle = \int_{\mathbb{R}^3} T(\psi) \cdot \bar{\psi} dx$$

*which is called “sandwiching” formula, with the operators*

$$x \quad , \quad -\frac{i\hbar}{m}\nabla \quad , \quad -i\hbar\nabla \quad , \quad -\frac{\hbar^2\Delta}{2m} \quad , \quad -\frac{\hbar^2\Delta}{2m} + V$$

*representing the position, speed, momentum, kinetic energy, and total energy.*

In other words, we are doing here two things. First, we are declaring by axiom that various “sandwiching” formulae found before by Heisenberg, involving the operators at the end, that we will not get into in detail here, hold true. And second, we are raising the possibility for other quantum mechanical systems, more complicated, to be described as well by the mathematics of the operators on a certain Hilbert space  $H$ , as above.

So, this was the story of early quantum mechanics, over-simplified as to fit here in a few pages. For more, you can check Feynman [34] for foundations and everything, including for some nice pictures and explanations regarding Fact 1.21. You have as well Griffiths [43] or Weinberg [94], for further explanations on Definition 1.23, not to forget Dirac’s original text [29], and all this is discussed as well in my book [7].

Now with this in hand, we can solve indeed the hydrogen atom, as follows:

**THEOREM 1.24.** *Hydrogen and other atoms are formed by a core of protons and neutrons, surrounded by a cloud of electrons, basically obeying to a modified version of electromagnetism. And with a fine mechanism involved, as follows:*

- (1) *The electrons are free to move only on certain specified elliptic orbits, labelled  $1, 2, 3, \dots$ , situated at certain specific heights.*
- (2) *The electrons can jump or fall between orbits  $n_1 < n_2$ , absorbing or emitting light and heat, that is, electromagnetic waves, as accelerating charges.*
- (3) *The energy of such a wave, coming from  $n_1 \rightarrow n_2$  or  $n_2 \rightarrow n_1$ , is given, via the Planck viewpoint, by the Rydberg formula, applied with  $n_1 < n_2$ .*
- (4) *The simplest such jumps are those observed by Lyman, Balmer, Paschen. And multiple jumps explain the Ritz-Rydberg formula.*

**PROOF.** There is a long story with all this, which simplified, is as follows:

(1) The statement, in its conjectural form, is due to Bohr, who was the initiator of the whole program. With the comment that, while all this is very familiar to us, nowadays, at that time, beginning of the 20th century, this was truly revolutionary.

(2) More precisely, Bohr came upon this by putting together a dazzling amount of seemingly unrelated physics, coming on one hand from Lyman, Balmer, Paschen, on the other hand from Planck, and from Einstein too, but then also from some key bombarding experiments by Thomson and Rutherford, and also from the radioactivity findings of Becquerel and Pierre and Marie Curie. And putting all this together, in the above form, was probably one of the smartest things that ever happened, in the history of physics.

(3) However, Bohr was unable to prove his claim, due to difficulties with the mathematical modeling of all this, which at first thought should involve a suitable modification of the Maxwell equations, but with this idea leading in fact nowhere.

(4) But then, a young Heisenberg came with his Principle 1.19, and solved the problem. And with the comment that Heisenberg did not really know about matrices when he started his work, and had to reinvent part of matrix theory, for solving his problem. Which is just lovely, but not that uncommon, every now and then a young mathematician or physicist, who skipped some classes in school, comes with a huge new thing.

(5) A few years later Schrödinger, who was working on this too, came with his Claim 1.22, and solved the problem too, in a better way than Heisenberg.

(6) A few more years later Dirac axiomatized quantum mechanics, along the lines of Definition 1.23, closing the axiomatic discussion, at least for some time, and with part of the credit going to De Broglie, for his work on the dual particle/wave nature of the electron, and to Pauli and others too, for their work on the electron spin.

(7) However, let us mention that all this is a never-ending story, continuing up to the present day. Indeed, at the fine level, several corrections must be made to the above

statement, and skipping some details here, until someone comes with a mathematical formula for the fine structure constant,  $\alpha \simeq 1/137$ , things are not over with hydrogen.

(8) As for quantum mechanics in general, contradictions and paradoxes are accumulating over the time, rather than disappearing, to the despair of people seriously doing quantum mechanics, and to the delight of people not doing any, or doing some, but being relaxed about it. And with the first one to have conjectured this mess being Einstein. For more on all this, you have for instance the nice popular book of Kumar [59].  $\square$

As a conclusion now to all this, answering Question 1.10, we have:

ANSWER 1.25. *Yes, quantum physics is all about matrices  $A \in M_N(\mathbb{C})$ , which can be possibly infinite,  $N = \infty$ , and are often self-adjoint,  $A = A^*$ . And mathematical quantum spaces of type  $M_N$ , formally defined by  $C(M_N) = M_N(\mathbb{C})$ , can only help with this.*

And good news, done with the physics, at least for this opening chapter of the present book. We have our math problem, and in what follows we will have a look at spaces of type  $M_N$ , and more generally at unions of such spaces, and graph structures on them.

### 1c. Operator algebras

In order to axiomatize the quantum spaces, we first need to talk about operator algebras. Deviating a bit from what Heisenberg was saying, for some reasons to become clear later on, we will only need here bounded operators. We first have:

THEOREM 1.26. *The bounded operators  $T : H \rightarrow H$  which are bounded,*

$$\|T\| = \sup_{\|x\|=1} \|Tx\| < \infty$$

*form a complex algebra  $B(H)$ , which is complete with respect to this norm. In the case where the space  $H$  comes with a basis  $\{e_i\}_{i \in I}$ , we have an embedding*

$$B(H) \subset M_I(\mathbb{C})$$

*which is  $M_N(\mathbb{C}) \subset M_N(\mathbb{C})$  for  $H = \mathbb{C}^N$ , but which is not an isomorphism in general.*

PROOF. All this is standard, with the algebra property of  $B(H)$  being clear, with the norm property of  $\|\cdot\|$  being clear too, and with the norm closedness of  $B(H)$  coming by constructing the limit of a Cauchy sequence  $\{T_n\}$  as follows:

$$Tx = \lim_{n \rightarrow \infty} T_n x \quad , \quad \forall x \in H$$

Finally, in what regards the embedding  $B(H) \subset M_I(\mathbb{C})$ , this can be constructed by using the same formula as in usual linear algebra, namely:

$$T_{ij} = \langle T e_j, e_i \rangle$$



As for the fact that this embedding is not an isomorphism, when  $\dim H = \infty$ , the point here is that with  $I = \mathbb{N}$  the infinite matrix  $T = \text{diag}(0, 1, 2, 3, \dots)$  does not come from a bounded operator, providing us with the desired counterexample.  $\square$

Next in line, we have the following result:

**THEOREM 1.27.** *Any bounded operator  $T \in B(H)$  has an adjoint  $T^* \in B(H)$ , given by the following formula, valid for any two vectors  $x, y \in H$ :*

$$\langle Tx, y \rangle = \langle x, T^*y \rangle$$

The operation  $T \rightarrow T^*$  is then an isometric involution of  $B(H)$ , and we have:

$$\|TT^*\| = \|T\|^2$$

When  $H$  comes with an orthonormal basis  $\{e_i\}_{i \in I}$ , we have  $(T^*)_{ij} = \overline{T_{ji}}$ .

**PROOF.** As before, all this is standard material. Given an operator  $T \in B(H)$ , let us pick a vector  $y \in H$ , and consider the following linear form:

$$x \rightarrow \langle Tx, y \rangle$$

This linear form must then come from a scalar product with a vector  $T^*y$ , as in the statement, and we obtain in this way a definition for  $T^*$ , namely  $y \rightarrow T^*y$ . It is then routine to check that we have indeed  $T^* \in B(H)$ , with this coming from:

$$\|T^*\| = \|T\|$$

The fact that  $T \rightarrow T^*$  is then an involution of  $B(H)$  is routine too. Regarding now the formula  $\|TT^*\| = \|T\|^2$ , in one sense we have the following estimate:

$$\|TT^*\| \leq \|T\| \cdot \|T^*\| = \|T\|^2$$

In the other sense, we have the following estimate:

$$\begin{aligned} \|T\|^2 &= \sup_{\|x\|=1} |\langle Tx, Tx \rangle| \\ &= \sup_{\|x\|=1} |\langle x, T^*Tx \rangle| \\ &\leq \|T^*T\| \end{aligned}$$

Now by replacing in this formula  $T \rightarrow T^*$  we obtain  $\|T\|^2 \leq \|TT^*\|$ , as desired. Finally,  $(T^*)_{ij} = \overline{T_{ji}}$  is clear from the formula  $T_{ij} = \langle Te_j, e_i \rangle$ , applied to  $T, T^*$ .  $\square$

Good news, we can now talk about operator algebras, as follows:

**DEFINITION 1.28.** *An operator algebra is an algebra of bounded operators  $A \subset B(H)$  which contains the unit, is closed under taking adjoints,*

$$T \in A \implies T^* \in A$$

*and is closed as well under the norm.*

This definition is in fact one of the many possible ones, with the choice here being a matter of knowledge of mathematics, and physics, and taste. But more on this later. Getting now to where we wanted to get, with this, we can formulate some tough results, inspired by the usual linear algebra, that of the algebra  $M_N(\mathbb{C})$ , as follows:

**THEOREM 1.29.** *The following happen:*

- (1) *Any self-adjoint operator,  $T = T^*$ , is diagonalizable.*
- (2) *More generally, any normal operator,  $TT^* = T^*T$ , is diagonalizable.*
- (3) *In fact, any family  $\{T_i\}$  of commuting normal operators is diagonalizable.*

*Thus, any commutative operator algebra is of the form  $A = C(X)$ , with  $X$  compact space.*

**PROOF.** This is certainly a tough theorem, with (1,2,3) coming by generalizing the spectral theorem, in its various incarnations, for the usual matrices  $M \in M_N(\mathbb{C})$ . As for the final conclusion, this follows from (3), because if we write  $A = \text{span}(T_i)$ , then the family  $\{T_i\}$  consists of commuting normal operators, and this leads to the conclusion  $A = C(X)$ , with  $X$  being a certain compact space associated to the family  $\{T_i\}$ .  $\square$

In relation with the above result, there are some good news and some bad news. The good news first, we can, eventually, talk about quantum spaces, as follows:

**DEFINITION 1.30.** *We can think of any operator algebra  $A \subset B(H)$  as being of the form*

$$A = C(X)$$

*with  $X$  compact quantum space. When  $A$  is commutative,  $X$  is a usual compact space.*

As for the bad news, all this is based on Theorem 1.29, which remains something quite complicated, and that we would rather like to avoid, when building foundations. Also, there is a problem with functoriality, because a morphism a quantum spaces  $X \rightarrow Y$  should normally come from a morphism of algebras  $C(Y) \rightarrow C(X)$ , but shall we ask or not something in relation with the embeddings  $C(X) \subset B(H)$  and  $C(Y) \subset B(K)$ . And finally, we have a philosophical problem too, the Hilbert spaces are certainly nice objects, but do we really need them for talking about basic things like quantum spaces.

Summarizing, Definition 1.28, Theorem 1.29 and Definition 1.30 are good, but not ideal, so better find something else. And here is the magic trick, due to Gelfand:

**DEFINITION 1.31.** *An abstract operator algebra, or  $C^*$ -algebra, is a complex algebra  $A$  having a norm  $\|\cdot\|$  and an involution  $*$ , subject to the following conditions:*

- (1)  *$A$  is closed with respect to the norm.*
- (2) *We have  $\|aa^*\| = \|a\|^2$ , for any  $a \in A$ .*

In other words, what we did here is to axiomatize the abstract properties of the operator algebras  $A \subset B(H)$ , without any reference to the Hilbert space  $H$ . We will see in a moment that our axiomatization is indeed complete, in the sense that any  $C^*$ -algebra

appears as an operator algebra,  $A \subset B(H)$ . Thus, getting back now to our quantum space questions, we will be able to recycle Definition 1.30, simply by replacing there “operator algebra” by  $C^*$ -algebra, and everything, or almost, will be fine.

Getting to work now, let us develop the theory of  $C^*$ -algebras. We first have:

**THEOREM 1.32.** *Given an element  $a \in A$  of a  $C^*$ -algebra, define its spectrum as:*

$$\sigma(a) = \left\{ \lambda \in \mathbb{C} \mid a - \lambda \notin A^{-1} \right\}$$

*The following spectral theory results hold, exactly as in the  $A = B(H)$  case:*

- (1) *We have  $\sigma(ab) \cup \{0\} = \sigma(ba) \cup \{0\}$ .*
- (2) *We have  $\sigma(f(a)) = f(\sigma(a))$ , for any  $f \in \mathbb{C}(X)$  having poles outside  $\sigma(a)$ .*
- (3) *The spectrum  $\sigma(a)$  is compact, non-empty, and contained in  $D_0(\|a\|)$ .*
- (4) *The spectra of unitaries ( $u^* = u^{-1}$ ) and self-adjoints ( $a = a^*$ ) are on  $\mathbb{T}, \mathbb{R}$ .*
- (5) *The spectral radius of normal elements ( $aa^* = a^*a$ ) is given by  $\rho(a) = \|a\|$ .*

*In addition, assuming  $a \in A \subset B$ , the spectra of  $a$  with respect to  $A$  and to  $B$  coincide.*

**PROOF.** Here the assertions (1-5), which are of course formulated a bit informally, are well-known for the full operator algebra  $A = B(H)$ , and the proof in general is similar:

(1) Assuming that  $1 - ab$  is invertible, with inverse  $c$ , we have  $abc = cab = c - 1$ , and it follows that  $1 - ba$  is invertible too, with inverse  $1 + bca$ . Thus  $\sigma(ab), \sigma(ba)$  agree on  $1 \in \mathbb{C}$ , and by linearity, it follows that  $\sigma(ab), \sigma(ba)$  agree on any point  $\lambda \in \mathbb{C}^*$ .

(2) The formula  $\sigma(f(a)) = f(\sigma(a))$  is clear for polynomials,  $f \in \mathbb{C}[X]$ , by factorizing  $f - \lambda$ , with  $\lambda \in \mathbb{C}$ . Then, the extension to the rational functions is straightforward, because  $P(a)/Q(a) - \lambda$  is invertible precisely when  $P(a) - \lambda Q(a)$  is.

(3) By using  $1/(1 - b) = 1 + b + b^2 + \dots$  for  $\|b\| < 1$  we obtain that  $a - \lambda$  is invertible for  $|\lambda| > \|a\|$ , and so  $\sigma(a) \subset D_0(\|a\|)$ . It is also clear that  $\sigma(a)$  is closed, so what we have is a compact set. Finally, assuming  $\sigma(a) = \emptyset$  the function  $f(\lambda) = \varphi((a - \lambda)^{-1})$  is well-defined, for any  $\varphi \in A^*$ , and by Liouville we get  $f = 0$ , contradiction.

(4) Assuming  $u^* = u^{-1}$  we have  $\|u\| = 1$ , and so  $\sigma(u) \subset D_0(1)$ . But with  $f(z) = z^{-1}$  we obtain via (2) that we have as well  $\sigma(u) \subset f(D_0(1))$ , and this gives  $\sigma(u) \subset \mathbb{T}$ . As for the result regarding the self-adjoints, this can be obtained from the result for the unitaries, by using (2) with functions of type  $f(z) = (z + it)/(z - it)$ , with  $t \in \mathbb{R}$ .

(5) It is routine to check, by integrating quantities of type  $z^n/(z - a)$  over circles centered at the origin, and estimating, that the spectral radius is given by  $\rho(a) = \lim \|a^n\|^{1/n}$ . But in the self-adjoint case,  $a = a^*$ , this gives  $\rho(a) = \|a\|$ , by using exponents of type  $n = 2^k$ , and then the extension to the general normal case is straightforward.

(6) Regarding now the last assertion, the inclusion  $\sigma_B(a) \subset \sigma_A(a)$  is clear. For the converse, assume  $a - \lambda \in B^{-1}$ , and set  $b = (a - \lambda)^*(a - \lambda)$ . We have then:

$$\sigma_A(b) - \sigma_B(b) = \left\{ \mu \in \mathbb{C} - \sigma_B(b) \mid (b - \mu)^{-1} \in B - A \right\}$$

Thus this difference is an open subset of  $\mathbb{C}$ . On the other hand  $b$  being self-adjoint, its two spectra are both real, and so is their difference. Thus the two spectra of  $b$  are equal, and in particular  $b$  is invertible in  $A$ , and so  $a - \lambda \in A^{-1}$ , as desired.  $\square$

With these ingredients, we can now prove a key result, as follows:

**THEOREM 1.33 (Gelfand).** *If  $X$  is a compact space, the algebra  $C(X)$  of continuous functions on it  $f : X \rightarrow \mathbb{C}$  is a  $C^*$ -algebra, with usual norm and involution, namely:*

$$\|f\| = \sup_{x \in X} |f(x)| \quad , \quad f^*(x) = \overline{f(x)}$$

*Conversely, any commutative  $C^*$ -algebra is of this form,  $A = C(X)$ , with*

$$X = \left\{ \chi : A \rightarrow \mathbb{C} \text{ , normed algebra character} \right\}$$

*with topology making continuous the evaluation maps  $ev_a : \chi \rightarrow \chi(a)$ .*

**PROOF.** There are several things going on here, the idea being as follows:

(1) The first assertion is clear from definitions. Observe that we have indeed:

$$\|ff^*\| = \sup_{x \in X} |f(x)|^2 = \|f\|^2$$

Observe also that the algebra  $C(X)$  is commutative, because  $fg = gf$ .

(2) Conversely, given a commutative  $C^*$ -algebra  $A$ , let us define  $X$  as in the statement. Then  $X$  is compact, and  $a \rightarrow ev_a$  is a morphism of algebras, as follows:

$$ev : A \rightarrow C(X)$$

(3) We first prove that  $ev$  is involutive. We use the following formula, which is similar to the  $z = Re(z) + iIm(z)$  decomposition formula for usual complex numbers:

$$a = \frac{a + a^*}{2} + i \cdot \frac{a - a^*}{2i}$$

Thus it is enough to prove  $ev_{a^*} = ev_a^*$  for the self-adjoint elements  $a$ . But this is the same as proving that  $a = a^*$  implies that  $ev_a$  is a real function, which is in turn true, by Theorem 1.32, because  $ev_a(\chi) = \chi(a)$  is an element of  $\sigma(a)$ , contained in  $\mathbb{R}$ .

(4) Since  $A$  is commutative, each element is normal, so  $ev$  is isometric:

$$\|ev_a\| = \rho(a) = \|a\|$$

It remains to prove that  $ev$  is surjective. But this follows from the Stone-Weierstrass theorem, because  $ev(A)$  is a closed subalgebra of  $C(X)$ , which separates the points.  $\square$

The above result is something truly remarkable, and we can now formulate:

DEFINITION 1.34. *Given an arbitrary  $C^*$ -algebra  $A$ , we can formally write it as*

$$A = C(X)$$

*with  $X$  compact quantum space. When  $A$  is commutative,  $X$  is a usual compact space.*

Observe the similarity with Definition 1.30, which is now to be forgotten. As a last twist to the plot, however, a quick comparison between Theorem 1.29 and Theorem 1.33 suggests that operator algebra and  $C^*$ -algebra might be actually the same thing. And this is indeed the case, the result, due to Gelfand-Naimark-Segal, being as follows:

THEOREM 1.35 (GNS). *Any  $C^*$ -algebra appears as an operator algebra:*

$$A \subset B(H)$$

*Moreover, when  $A$  is separable, which is usually the case,  $H$  can be taken separable.*

PROOF. This comes as a continuation of Theorem 1.33, the idea being as follows:

(1) Let us first prove that the result holds in the commutative case,  $A = C(X)$ . Here, we can pick a positive measure on  $X$ , and construct our embedding as follows:

$$C(X) \subset B(L^2(X)) \quad , \quad f \rightarrow [g \rightarrow fg]$$

(2) In general the proof is similar, the idea being that given a  $C^*$ -algebra  $A$  we can construct a Hilbert space  $H = L^2(A)$ , and then an embedding as above:

$$A \subset B(L^2(A)) \quad , \quad a \rightarrow [b \rightarrow ab]$$

(3) Finally, the last assertion is clear, because when  $A$  is separable, meaning that it has a countable algebraic basis, so does the associated Hilbert space  $H = L^2(A)$ .  $\square$

As a conclusion, we have now a good notion of compact quantum space, coming from Theorem 1.33, tools for the study of such spaces, coming from Theorem 1.32, and even a theorem allowing us to pull out of a hat a Hilbert space, namely Theorem 1.35.

## 1d. Quantum spaces

In what follows, we will be mainly interested in finite quantum spaces. We have the following result, complementing the general  $C^*$ -algebra theory developed above:

THEOREM 1.36. *Let  $A$  be a finite dimensional  $*$ -algebra.*

- (1) *We can write  $1 = p_1 + \dots + p_k$ , with  $p_i \in A$  central minimal projections.*
- (2) *Each of the vector spaces  $A_i = p_i A p_i$  is a non-unital  $*$ -subalgebra of  $A$ .*
- (3) *We have a non-unital  $*$ -algebra sum decomposition  $A = A_1 \oplus \dots \oplus A_k$ .*
- (4) *We have unital  $*$ -algebra isomorphisms  $A_i \simeq M_{n_i}(\mathbb{C})$ , with  $n_i = \text{rank}(p_i)$ .*
- (5) *Thus, we have a  $*$ -algebra isomorphism  $A \simeq M_{n_1}(\mathbb{C}) \oplus \dots \oplus M_{n_k}(\mathbb{C})$ .*

PROOF. Let us first look at the center of our algebra,  $Z(A) = A \cap A'$ . It is elementary to prove that this center, as an algebra, is of the following form:

$$Z(A) \simeq \mathbb{C}^k$$

Consider now the standard basis  $e_1, \dots, e_k \in \mathbb{C}^k$ , and let  $p_1, \dots, p_k \in Z(A)$  be the images of these vectors via the above identification. In other words, these elements  $p_1, \dots, p_k \in A$  are central minimal projections, summing up to 1:

$$p_1 + \dots + p_k = 1$$

The idea is then that this partition of the unity will eventually lead to the block decomposition of  $A$ , as in the statement. We prove this in 3 steps, as follows:

Step 1. We first construct the matrix blocks, our claim here being that each of the following linear subspaces of  $A$  are non-unital  $*$ -subalgebras of  $A$ :

$$A_i = p_i A p_i$$

But this is clear, with the fact that each  $A_i$  is closed under the various non-unital  $*$ -subalgebra operations coming from the projection equations  $p_i = p_i^* = p_i^2$ .

Step 2. We prove now that the above algebras  $A_i \subset A$  are in a direct sum position, in the sense that we have a non-unital  $*$ -algebra sum decomposition, as follows:

$$A = A_1 \oplus \dots \oplus A_k$$

As with any direct sum question, we have two things to be proved here. First, by using the formula  $p_1 + \dots + p_k = 1$  and the projection equations  $p_i = p_i^* = p_i^2$ , we conclude that we have the needed generation property, namely:

$$A_1 + \dots + A_k = A$$

As for the fact that the sum is indeed direct, this follows as well from the formula  $p_1 + \dots + p_k = 1$ , and from the projection equations  $p_i^2 = p_i = p_i^*$ .

Step 3. Our claim now, which will finish the proof, is that each of the  $*$ -subalgebras  $A_i = p_i A p_i$  constructed above is a full matrix algebra. To be more precise here, with  $n_i = \text{rank}(p_i)$ , our claim is that we have isomorphisms, as follows:

$$A_i \simeq M_{n_i}(\mathbb{C})$$

In order to prove this claim, recall that the projections  $p_i \in A$  were chosen central and minimal. Thus, the center of each of the algebras  $A_i$  reduces to the scalars:

$$Z(A_i) = \mathbb{C}$$

But this shows that each of the algebras  $A_i$  is a full matrix algebra, and by putting now everything together we obtain  $A \simeq M_{n_1}(\mathbb{C}) \oplus \dots \oplus M_{n_k}(\mathbb{C})$ , as desired.  $\square$

Good news, we have now all the needed tools in our bag for getting back to Speculations 1.5, 1.6, 1.7, 1.8, and eating them raw. First, we have the following definition:

DEFINITION 1.37. *A finite quantum space  $F$  is the abstract dual of a finite dimensional  $C^*$ -algebra  $A$ , according to the following formula:*

$$C(F) = A$$

*The formal number of elements of such a space is  $|F| = \dim A$ . By decomposing the algebra  $A$ , we have a formula of the following type:*

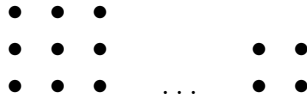
$$C(F) = M_{n_1}(\mathbb{C}) \oplus \dots \oplus M_{n_k}(\mathbb{C})$$

*With  $n_1 = \dots = n_k = 1$  we obtain in this way the space  $F = \{1, \dots, k\}$ . Also, when  $k = 1$  the equation is  $C(F) = M_n(\mathbb{C})$ , and the solution will be denoted  $F = M_n$ .*

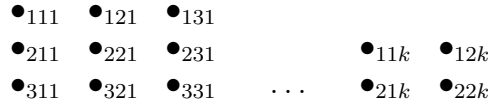
As a first observation, by decomposing the algebra  $A$  as a sum of matrix algebras, as above, we have the following formula for the formal number of points:

$$|F| = n_1^2 + \dots + n_k^2$$

Pictorially, this suggests representing  $F$  as a set of  $|F|$  points in the plane, arranged in squares having sides  $n_1, \dots, n_k$ , coming from the matrix blocks of  $A$ , as follows:



However, this picture is not exactly correct, because the above points are not true, classical points. In order to fix this, the best is to label the points, as follows:



But this convention is perhaps a bit too heavy. In practice, we have in fact 3 possible conventions, that we will all use, depending on the setting, which are as follows:

DEFINITION 1.38. *Given a finite quantum space  $F$ , coming via a formula of type  $C(F) = M_{n_1}(\mathbb{C}) \oplus \dots \oplus M_{n_k}(\mathbb{C})$ , we have the following conventions for drawing  $F$ :*

- (1) *Triple indices.* We represent  $F$  as a set of  $N = |F|$  points, with each point being decorated with a triple index  $ija$ , coming from the standard basis  $\{e_{ij}^a\} \subset A$ .
- (2) *Double indices.* As before, but by ignoring the index  $a$ , with the convention that  $i, j$  belong to various indexing sets, one for each of the matrix blocks of  $A$ .
- (3) *Single indices.* As before, but with each point being now decorated with a single index, playing the role of the previous triple indices  $ija$ , or double indices  $ij$ .

And with this, we have basically converted Speculations 1.5, 1.6, 1.7 into rigorous mathematics. As for Speculation 1.8, this can be made rigorous too, as follows:

DEFINITION 1.39. *Given a finite quantum space  $F$ , we construct the functional*

$$tr : C(F) \rightarrow B(l^2(F)) \rightarrow \mathbb{C}$$

*obtained by applying the regular representation, and the normalized matrix trace, and we call it integration with respect to the normalized counting measure on  $F$ .*

To be more precise, consider the algebra  $A = C(F)$ , which is by definition finite dimensional. We can make act  $A$  on itself, by left multiplication:

$$\pi : A \rightarrow \mathcal{L}(A) \quad , \quad a \rightarrow (b \rightarrow ab)$$

The target of  $\pi$  being a matrix algebra,  $\mathcal{L}(A) \simeq M_N(\mathbb{C})$  with  $N = \dim A$ , we can further compose with the normalized matrix trace, and we obtain  $tr$ :

$$tr = \frac{1}{N} Tr \circ \pi$$

As basic examples, for both  $F = \{1, \dots, N\}$  and  $F = M_N$  we obtain the usual trace. In general, with  $C(F) = M_{n_1}(\mathbb{C}) \oplus \dots \oplus M_{n_k}(\mathbb{C})$ , the weights of  $tr$  are:

$$c_i = \frac{n_i^2}{\sum_i n_i^2}$$

To conclude now, we have a rigorous definition for finite quantum spaces, and some pictures for them, which are rigorous too. With respect to our original Speculations 1.5, 1.6, 1.7, 1.8, everything there lies now on a rigorous basis, and we will leave the few details to be checked, namely those regarding the twisting matters, as an exercise, below.

### 1e. Exercises

We had an exciting chapter, mixing a bit of everything, mathematics and physics, for all audiences, and as exercises on this, for all audiences too, we hope, we have:

EXERCISE 1.40. *Diagonalizable matrices are dense, via  $\Delta(P_A)$ , or Jordan form.*

EXERCISE 1.41. *Learn the spectral theorem for normal matrices,  $AA^* = A^*A$ .*

EXERCISE 1.42. *Learn the Maxwell equations, and the mechanism of light creation.*

EXERCISE 1.43. *Learn optics, including the Fourier decomposition of wave packets.*

EXERCISE 1.44. *Read, during a week-end, the popular book “Quantum” by Kumar.*

EXERCISE 1.45. *Learn more operator algebras, including full proof of GNS.*

EXERCISE 1.46. *Clarify what happens to the norm, in  $A \simeq M_{n_1}(\mathbb{C}) \oplus \dots \oplus M_{n_k}(\mathbb{C})$ .*

EXERCISE 1.47. *Have some fun in axiomatizing the twisting  $M_2 \sim \{1, 2, 3, 4\}$ .*

As bonus exercise, hard as bonus exercises go, learn some quantum mechanics, the standard references here being Feynman [34], Griffiths [43] and Weinberg [94].



## CHAPTER 2

### Quantum graphs

#### 2a. Quantum graphs

We have the following straightforward extension of the usual notion of finite graph, obtained by using a finite quantum space as set of vertices:

DEFINITION 2.1. We call “finite quantum graph” a pair of type

$$X = (F, d)$$

with  $F$  being a finite quantum space, and with  $d \in M_N(\mathbb{C})$  being a matrix.

This is of course something quite general. In the case  $F = \{1, \dots, N\}$  for instance, what we have here is a directed graph, with the edges  $i \rightarrow j$  colored by complex numbers  $d_{ij} \in \mathbb{C}$ , and with self-edges  $i \rightarrow i$  allowed too, again colored by numbers  $d_{ii} \in \mathbb{C}$ . In the general case, however, where  $F$  is arbitrary, the need for extra conditions of type  $d = d^*$ , or  $d_{ii} = 0$ , or  $d \in M_N(\mathbb{R})$ , or  $d \in M_N(0, 1)$  and so on, is not very natural, as we will soon discover, and it is best to use Definition 2.1 as such, with no restrictions on  $d$ .

In general, a quantum graph can be represented as a colored oriented graph on  $\{1, \dots, N\}$ , where  $N = |F|$ , with the vertices being decorated by single indices  $i$ , and with the colors being complex numbers, namely the entries of  $d$ . This is similar to the formalism from before, but there is a discussion here in what regards the exact choice of the colors, which are usually irrelevant in connection with our symmetry problematics, and so can be true colors instead of complex numbers. More on this later.

#### 2b. Symmetry groups

In order to construct the symmetry groups  $G(X)$  of our quantum graphs  $X$ , let us first review the symmetry group theory for the usual graphs. For reasons that will become clear later, it is convenient to use a functional analytic approach to this, based on:

THEOREM 2.2. Given a permutation group  $G \subset S_N \subset O_N$ , the standard coordinates of the group elements,  $u_{ij}(g) = g_{ij}$ , are given by:

$$u_{ij} = \chi \left( \sigma \in G \mid \sigma(j) = i \right)$$

Moreover, these coordinate functions  $u_{ij} : G \rightarrow \mathbb{C}$  generate the algebra  $C(G)$ .

PROOF. Here the first assertion comes from the fact that the entries of the permutation matrices  $\sigma \in S_N \subset O_N$ , acting as  $\sigma(e_i) = e_{\sigma(i)}$ , are given by the following formula:

$$\sigma_{ij} = \begin{cases} 1 & \text{if } \sigma(j) = i \\ 0 & \text{otherwise} \end{cases}$$

As for the second assertion, this comes from the Stone-Weierstrass theorem, because the coordinate functions  $u_{ij} : G \rightarrow \mathbb{C}$  obviously separate the group elements  $\sigma \in G$ .  $\square$

We are led in this way to the following definition:

DEFINITION 2.3. *The magic matrix associated to a subgroup  $G \subset S_N$  is the  $N \times N$  matrix of characteristic functions*

$$u_{ij} = \chi \left( \sigma \in G \mid \sigma(j) = i \right)$$

with the name “magic” coming from the fact that, on each row and each column, these characteristic functions sum up to 1.

The interest in this notion comes from the fact, that we know from Theorem 2.2, that the entries of the magic matrix generate the algebra of functions on our group:

$$C(G) = \langle u_{ij} \rangle$$

We will talk more in detail later about such matrices, and their correspondence with the subgroups  $G \subset S_N$ , and what can be done with it, in the general framework of representation theory. However, for making our point, here is the general principle:

PRINCIPLE 2.4. *Everything that you can do with your group  $G \subset S_N$  can be expressed in terms of the magic matrix  $u = (u_{ij})$ , quite often with good results.*

This principle comes from the above Stone-Weierstrass result,  $C(G) = \langle u_{ij} \rangle$ . Indeed, when coupled with some basic spectral theory, and more specifically with the Gelfand theorem from operator algebras, this result tells us that our group  $G$  appears as the spectrum of the algebra  $\langle u_{ij} \rangle$ , therefore leading to the above principle.

As an illustration for all this, in relation with the graphs, we have:

THEOREM 2.5. *Given a subgroup  $G \subset S_N$ , the transpose of its action map  $X \times G \rightarrow X$  on the set  $X = \{1, \dots, N\}$ , given by  $(i, \sigma) \rightarrow \sigma(i)$ , is given by:*

$$\Phi(e_i) = \sum_j e_j \otimes u_{ji}$$

Also, in the case where we have a graph with  $N$  vertices, the action of  $G$  on the vertex set  $X$  leaves invariant the edges precisely when we have

$$du = ud$$

with  $d$  being as usual the adjacency matrix of the graph.

PROOF. There are several things going on here, the idea being as follows:

(1) Given a subgroup  $G \subset S_N$ , if we set  $X = \{1, \dots, N\}$ , we have indeed an action map as follows, and with the reasons of using  $X \times G$  instead of the perhaps more familiar  $G \times X$  being dictated by some quantum algebra, that we will do later in this book:

$$a : X \times G \rightarrow X \quad , \quad a(i, \sigma) = \sigma(i)$$

(2) Now by transposing this map, we obtain a morphism of algebras, as follows:

$$\Phi : C(X) \rightarrow C(X) \otimes C(G) \quad , \quad \Phi(f)(i, \sigma) = f(\sigma(i))$$

When evaluated on the Dirac masses, this map  $\Phi$  is then given by:

$$\Phi(e_i)(j, \sigma) = e_i(\sigma(j)) = \delta_{\sigma(j)i}$$

Thus, in tensor product notation, we have the following formula, as desired:

$$\Phi(e_i)(j, \sigma) = \left( \sum_j e_j \otimes u_{ji} \right) (j, \sigma)$$

(3) Regarding now the second assertion, observe first that we have:

$$(du)_{ij}(\sigma) = \sum_k d_{ik} u_{kj}(\sigma) = \sum_k d_{ik} \delta_{\sigma(j)k} = d_{i\sigma(j)}$$

On the other hand, we have as well the following formula:

$$(ud)_{ij}(\sigma) = \sum_k u_{ik}(\sigma) d_{kj} = \sum_k \delta_{\sigma(k)i} d_{kj} = d_{\sigma^{-1}(i)j}$$

Thus  $du = ud$  reformulates as  $d_{ij} = d_{\sigma(i)\sigma(j)}$ , which gives the result.  $\square$

We have the following result, further building on the above:

**THEOREM 2.6.** *The symmetry group  $G(X)$  of a graph  $X$  having  $N$  vertices is given by the following formula, at the level of the corresponding algebra of functions,*

$$C(G(X)) = C(S_N) / \left\langle [u, d] = 0 \right\rangle$$

with  $d \in M_N(0, 1)$  being as usual the adjacency matrix of  $X$ .

PROOF. This follows indeed from Theorem 2.5, and more specifically, is just an abstract reformulation of the last assertion there.  $\square$

So long for magic unitaries, and their basic properties, and we will be back to this, on several occasions, in what follows. In fact, the magic matrices will get increasingly important, as the present book develops, because not far away from now, when starting to talk about the quantum permutation groups  $G$ , and their actions on the graphs  $X$ , these beasts will not really exist, as concrete objects  $G$ , but their associated magic matrices  $u = (u_{ij})$  will exist, and we will base our whole study on them. More on this later.

Getting back now to the quantum graphs  $X = (F, d)$ , we first need to talk about the symmetry groups  $S_F$  of the quantum spaces  $F$ . Following Wang [91], we have:

**DEFINITION 2.7.** *Given a finite quantum space  $F$ , we let  $\{e_i\}$  be the standard basis of  $B = C(F)$ , so that the multiplication, involution and unit of  $B$  are given by*

$$e_i e_j = e_{ij} \quad , \quad e_i^* = e_{\bar{i}} \quad , \quad 1 = \sum_{i=\bar{i}} e_i$$

where  $(i, j) \rightarrow ij$  is the standard partially defined multiplication on the indices, with the convention  $e_\emptyset = 0$ , and where  $i \rightarrow \bar{i}$  is the standard involution on the indices.

To be more precise, let  $\{e_{ab}^r\} \subset B$  be the multimatrix basis. We set  $i = (abr)$ , and with this convention, the multiplication, coming from  $e_{ab}^r e_{cd}^p = \delta_{rp} \delta_{bc} e_{ad}^r$ , is given by:

$$(abr)(cdp) = \begin{cases} (adr) & \text{if } b = c, r = p \\ \emptyset & \text{otherwise} \end{cases}$$

As for the involution, coming from  $(e_{ab}^r)^* = e_{ba}^r$ , this is given by:

$$\overline{(a, b, r)} = (b, a, r)$$

Finally, the unit formula comes from the following formula for the unit  $1 \in B$ :

$$1 = \sum_{ar} e_{aa}^r$$

Regarding now the generalized quantum permutation groups  $S_F^+$ , the construction in Theorem 2.2 reformulates as follows, by using the above formalism:

**THEOREM 2.8.** *Given a finite quantum space  $F$ , with basis  $\{e_i\} \subset C(F)$  as above, the algebra  $C(S_F)$  is generated by commuting variables  $u_{ij}$  with the following relations,*

$$\begin{aligned} \sum_{ij=p} u_{ik} u_{jl} &= u_{p,kl} \quad , \quad \sum_{kl=p} u_{ik} u_{jl} = u_{ij,p} \\ \sum_{i=\bar{i}} u_{ij} &= \delta_{j\bar{j}} \quad , \quad \sum_{j=\bar{j}} u_{ij} = \delta_{i\bar{i}} \\ u_{ij}^* &= u_{\bar{i}\bar{j}} \end{aligned}$$

with the fundamental corepresentation being the matrix  $u = (u_{ij})$ . We call a matrix  $u = (u_{ij})$  satisfying the above relations “generalized magic”.

**PROOF.** It is routine to see that the algebra  $C(S_F)$  appears as follows, where  $N = |F|$ , and where  $\mu, \eta$  are the multiplication and unit maps of  $C(F)$ :

$$C(S_F) = C(U_N) / \left\langle \mu \in \text{Hom}(u^{\otimes 2}, u), \eta \in \text{Fix}(u) \right\rangle$$

But the relations  $\mu \in \text{Hom}(u^{\otimes 2}, u)$  and  $\eta \in \text{Fix}(u)$  produce the 1st and 4th relations in the statement, then the biunitarity of  $u$  gives the 5th relation, and finally the 2nd and 3rd relations follow from the 1st and 4th relations, by using the antipode.  $\square$

As an illustration, consider the case  $F = \{1, \dots, N\}$ . Here the index multiplication is  $ii = i$  and  $ij = \emptyset$  for  $i \neq j$ , and the involution is  $\bar{i} = i$ . Thus, our relations are as follows, corresponding to the standard magic conditions on a matrix  $u = (u_{ij})$ :

$$\begin{aligned} u_{ik}u_{il} &= \delta_{kl}u_{ik} \quad , \quad u_{ik}u_{jk} = \delta_{ij}u_{ik} \\ \sum_i u_{ij} &= 1 \quad , \quad \sum_j u_{ij} = 1 \\ u_{ij}^* &= u_{ij} \end{aligned}$$

As a second illustration now, which is something new, we have:

**THEOREM 2.9.** *For the space  $F = M_2$ , coming via  $C(F) = M_2(\mathbb{C})$ , we have*

$$S_F = SO_3$$

*with the action  $SO_3 \curvearrowright M_2(\mathbb{C})$  being the standard one, coming from  $SU_2 \rightarrow SO_3$ .*

**PROOF.** We have an action by conjugation  $SU_2 \curvearrowright M_2(\mathbb{C})$ , and this action produces, via the canonical quotient map  $SU_2 \rightarrow SO_3$ , an action as follows:

$$SO_3 \curvearrowright M_2(\mathbb{C})$$

But this action is easily seen to be universal, as claimed.  $\square$

Time now to get back to the quantum graphs. We have here:

**DEFINITION 2.10.** *The symmetry group of a graph  $X = (F, d)$  is the subgroup*

$$G(X) \subset S_F$$

*obtained via the relation  $du = ud$ , where  $u = (u_{ij})$  is the fundamental corepresentation.*

This is something very natural, coming as a continuation of the constructions for the usual graphs. We will see many explicit computations, in what follows. As a first observation, for the empty graph on a finite quantum space  $F$ , we certainly have:

$$G(X) = S_F$$

This is of course something trivial, but as shown by Theorem 2.9, the computation of  $S_F$  can be something quite tricky, leading us into Lie groups, and other pieces of subtle mathematics. As a second result here, further building on Theorem 2.9, we have:

**THEOREM 2.11.** *The classical symmetry group of  $F = M_K \times \{1, \dots, L\}$  is*

$$S_F = PU_K \wr S_L$$

*with on the right a wreath product, equal by definition to  $PU_K^L \rtimes S_L$ .*

PROOF. The fact that we have indeed an inclusion  $PU_K \wr S_L \subset S_F$  is standard. As for the fact that this inclusion  $PU_K \wr S_L \subset S_F$  is an isomorphism, this can be proved by picking an arbitrary element  $g \in S_F$ , and decomposing it.  $\square$

Observe that, as shown by Theorem 2.9, things are not over with the above result, because the group  $PU_K$  can be subject to some further study, and at  $K = 2$  for instance, we have an isomorphism  $PU_2 = SO_3$ . We will be back to this.

### 2c. The simplex

As a first piece of general theory, let us discuss now the simplices, in the quantum graph setting. You would say that this is something trivial, just draw edges everywhere, between all vertices, and you have your simplex. But, wait for it.

As we will soon discover, things are quite tricky here, leading us in particular to the conclusion that the simplex based on an arbitrary finite quantum space  $F$  is not a usual graph, with  $d \in M_N(0, 1)$  where  $N = |F|$ , but rather a sort of “signed graph”, with  $d \in M_N(-1, 0, 1)$ . Let us start our study with the following fact:

THEOREM 2.12. *Given a finite quantum space  $F$ , we have*

$$G(F_{empty}) = G(F_{full}) = S_F$$

where  $F_{empty}$  is the empty graph on the vertex set  $F$ , coming from the matrix  $d = 0$ , and where  $F_{full}$  is the simplex on the vertex set  $F$ , coming from the matrix

$$d = NP_1 - 1_N$$

where  $N = |F|$ , and where  $P_1$  is the orthogonal projection on the unit  $1 \in C(F)$ .

PROOF. This is something quite tricky, the idea being as follows:

(1) First of all, the formula  $G(F_{empty}) = S_F$  is clear from definitions, because the commutation of  $u$  with the matrix  $d = 0$  is automatic.

(2) Regarding  $G(F_{full}) = S_F$ , let us first discuss the classical case,  $F = \{1, \dots, N\}$ . Here the simplex  $F_{full}$  is the graph having having edges between any two vertices, whose adjacency matrix is  $d = \mathbb{I}_N - 1_N$ , where  $\mathbb{I}_N$  is the all-1 matrix. The commutation of  $u$  with  $1_N$  being automatic, and the commutation with  $\mathbb{I}_N$  being automatic too,  $u$  being bistochastic, we have  $[u, d] = 0$ , and so  $G(F_{full}) = S_F$  in this case, as stated.

(3) In the general case now, we know from the above that we have  $\eta \in \text{Fix}(u)$ , with  $\eta : \mathbb{C} \rightarrow C(F)$  being the unit map. Thus we have  $P_1 \in \text{End}(u)$ , and so the condition  $[u, P_1] = 0$  is automatic. Together with the fact that in the classical case we have  $\mathbb{I}_N = NP_1$ , this suggests to define the adjacency matrix of the simplex as being  $d = NP_1 - 1_N$ , and with this definition, we have indeed  $G(F_{full}) = S_F$ , as claimed.  $\square$

Let us study now the simplices  $F_{full}$  found in Theorem 2.12. In the classical case,  $F = \{1, \dots, N\}$ , what we have is of course the usual simplex. However, in the general case things are more mysterious, the first result here being as follows:

**PROPOSITION 2.13.** *The adjacency matrix of the simplex  $F_{full}$ , given by definition by  $d = NP_1 - 1_N$ , is a matrix  $d \in M_N(-1, 0, 1)$ , which can be computed as follows:*

- (1) *In single index notation,  $d_{ij} = \delta_{\bar{i}\bar{i}}\delta_{\bar{j}\bar{j}} - \delta_{ij}$ .*
- (2) *In double index notation,  $d_{ab,cd} = \delta_{ab}\delta_{cd} - \delta_{ac}\delta_{bd}$ .*
- (3) *In triple index notation,  $d_{abp,cdq} = \delta_{ab}\delta_{cd} - \delta_{ac}\delta_{bd}\delta_{pq}$ .*

**PROOF.** According to our single index conventions, from Definition 2.7, the adjacency matrix of the simplex is the one in the statement, namely:

$$\begin{aligned} d_{ij} &= (NP_1 - 1_N)_{ij} \\ &= \bar{1}_i \bar{1}_j - \delta_{ij} \\ &= \delta_{\bar{i}\bar{i}}\delta_{\bar{j}\bar{j}} - \delta_{ij} \end{aligned}$$

In double index notation now, with  $i = (ab)$  and  $j = (cd)$ , and  $a, b, c, d$  being usual matrix indices, each thought to be attached to the corresponding matrix block of  $C(F)$ , the formula that we obtain in the second one in the statement, namely:

$$\begin{aligned} d_{ab,cd} &= \delta_{ab,ba}\delta_{cd,dc} - \delta_{ab,cd} \\ &= \delta_{ab}\delta_{cd} - \delta_{ac}\delta_{bd} \end{aligned}$$

Finally, in standard triple index notation,  $i = (abp)$  and  $j = (cdq)$ , with  $a, b, c, d$  being now usual numeric matrix indices, ranging in  $1, 2, 3, \dots$ , and with  $p, q$  standing for corresponding blocks of the algebra  $C(F)$ , the formula that we obtain is:

$$\begin{aligned} d_{abp,cdq} &= \delta_{abp,bap}\delta_{cdq,dcq} - \delta_{abp,cdq} \\ &= \delta_{ab}\delta_{cd} - \delta_{ac}\delta_{bd}\delta_{pq} \end{aligned}$$

Thus, we are led to the conclusions in the statement.  $\square$

At the level of examples, for  $F = \{1, \dots, N\}$  the best is to use the above formula (1). The involution on the index set is  $\bar{\bar{i}} = i$ , and we obtain, as we should:

$$d_{ij} = 1 - \delta_{ij}$$

As a more interesting example now, for the quantum space  $F = M_n$ , coming by definition via the formula  $C(F) = M_n(\mathbb{C})$ , the situation is as follows:

**PROPOSITION 2.14.** *The simplex  $F_{full}$  with  $F = M_n$  is as follows:*

- (1) *The vertices are  $n^2$  points in the plane, arranged in square form.*
- (2) *Usual edges, worth 1, are drawn between distinct points on the diagonal.*
- (3) *In addition, each off-diagonal point comes with a self-edge, worth  $-1$ .*

PROOF. Here the most convenient is to use the double index formula from Proposition 2.13 (2), which tells us that  $d$  is as follows, with indices  $a, b, c, d \in \{1, \dots, n\}$ :

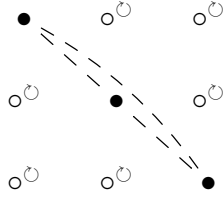
$$d_{ab,cd} = \delta_{ab}\delta_{cd} - \delta_{ac}\delta_{bd}$$

This quantity can be  $-1, 0, 1$ , and the study goes as follows:

– Case  $d_{ab,cd} = 1$ . This can only happen when  $\delta_{ab}\delta_{cd} = 1$  and  $\delta_{ac}\delta_{bd} = 0$ , corresponding to a formula of type  $d_{aa,cc} = 0$ , with  $a \neq c$ , and so to the edges in (2).

– Case  $d_{ab,cd} = -1$ . This can only happen when  $\delta_{ab}\delta_{cd} = 0$  and  $\delta_{ac}\delta_{bd} = 1$ , corresponding to a formula of type  $d_{ab,ab} = 0$ , with  $a \neq b$ , and so to the self-edges in (3).  $\square$

The above result is quite interesting, and as an illustration, here is the pictorial representation of the simplex  $F_{full}$  on the vertex set  $F = M_3$ , with the convention that the solid arrows are worth  $-1$ , and the dashed arrows are worth  $1$ :



More generally, we can in fact compute  $F_{full}$  for any finite quantum space  $F$ , with the result here, which will be our final saying on the subject, being as follows:

**THEOREM 2.15.** *Consider a finite quantum space  $F$ , and write it as follows, according to the decomposition formula  $C(F) = M_{n_1}(\mathbb{C}) \oplus \dots \oplus M_{n_k}(\mathbb{C})$  for its function algebra:*

$$F = M_{n_1} \sqcup \dots \sqcup M_{n_k}$$

*The simplex  $F_{full}$  is then the classical simplex formed by the points lying on the diagonals of  $M_{n_1}, \dots, M_{n_k}$ , with self-edges added, each worth  $-1$ , at the non-diagonal points.*

PROOF. The study here is quite similar to the one from the proof of Proposition 2.14, but by using this time the triple index formula from Proposition 2.13 (3), namely:

$$d_{abp,cdq} = \delta_{ab}\delta_{cd} - \delta_{ac}\delta_{bd}\delta_{pq}$$

Indeed, this quantity can be  $-1, 0, 1$ , and the  $1$  case appears precisely as follows, leading to the classical simplex mentioned in the statement:

$$d_{aap,ccq} = 1 \quad , \quad \forall ap \neq cq$$

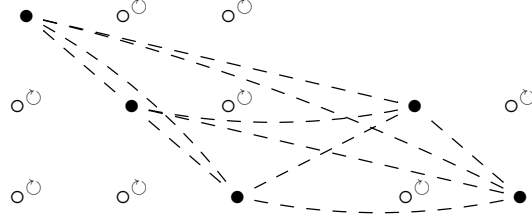
As for the remaining  $-1$  case, this appears precisely as follows, leading this time to the self-edges worth  $-1$ , also mentioned in the statement:

$$d_{abp,abp} = 1 \quad , \quad \forall a \neq b$$

Thus, we are led to the conclusion in the statement.  $\square$



As an illustration, here is the simplex on the vertex set  $F = M_3 \sqcup M_2$ , with again the convention that the solid arrows are worth  $-1$ , and the dashed arrows are worth  $1$ :



Long story short, we know what the simplex  $F_{full}$  is, and we have the formula  $G(F_{empty}) = G(F_{full}) = S_F$ , exactly as in the  $F = \{1, \dots, N\}$  case. Now with the above results in hand, we can talk as well about complementation, as follows:

**THEOREM 2.16.** *For any finite quantum graph  $X$  we have the formula*

$$G^+(X) = G^+(X^c)$$

where  $X \rightarrow X^c$  is the complementation operation, given by  $d_X + d_{X^c} = d_{F_{full}}$ .

**PROOF.** This follows from Theorem 2.12, and more specifically from the following commutation relation, which is automatic, as explained there:

$$[u, d_{F_{full}}] = 0$$

Let us mention too that, in what concerns the pictorial representation of  $X^c$ , this can be deduced from what we have Theorem 2.15, in the obvious way.  $\square$

## 2d. Further examples

In order to construct further examples of quantum graphs, let us start with:

**DEFINITION 2.17.** *A fibration of finite quantum spaces  $F \rightarrow E$  corresponds to an inclusion of finite dimensional  $C^*$ -algebras*

$$C(E) \subset C(F)$$

which is Markov, in the sense that it commutes with the canonical traces.

Here the commutation condition with the canonical traces means that the composition  $C(E) \subset C(F) \rightarrow \mathbb{C}$  should equal the canonical trace  $C(E) \rightarrow \mathbb{C}$ . At the level of the corresponding quantum spaces, this means that the quotient map  $F \rightarrow E$  must commute with the corresponding counting measures, and this is where our term ‘‘fibration’’ comes from. In order to talk now about the symmetry groups  $S_{F \rightarrow E}$ , we will need:

**PROPOSITION 2.18.** *Given a fibration  $F \rightarrow E$ , a closed subgroup  $G \subset S_F$  leaves invariant  $E$  precisely when its magic unitary  $u = (u_{ij})$  satisfies the condition*

$$e \in \text{End}(u)$$

where  $e : C(F) \rightarrow C(F)$  is the Jones projection, onto the subalgebra  $C(E) \subset C(F)$ .

PROOF. This is something that we know well, in the commutative case, where  $E$  is a usual finite set, and the proof in general is similar.  $\square$

We can now talk about twisted reflection groups, as follows:

THEOREM 2.19. *Any fibration of finite quantum spaces  $F \rightarrow E$  has a symmetry group, which is the biggest acting on  $E$  by leaving  $F$  invariant:*

$$S_{F \rightarrow E} \subset S_F$$

*At the level of algebras of functions, this symmetry group  $S_{F \rightarrow E}$  is obtained as follows, with  $e : C(F) \rightarrow C(E)$  being the Jones projection:*

$$C(S_{F \rightarrow E}) = C(S_F) / \langle e \in \text{End}(u) \rangle$$

*We call these groups  $S_{F \rightarrow E}$  twisted reflection groups.*

PROOF. This follows indeed from Proposition 2.18.  $\square$

Many things can be said, about the above quantum graphs and symmetry groups.

## 2e. Exercises

Exercises:

EXERCISE 2.20.

EXERCISE 2.21.

EXERCISE 2.22.

EXERCISE 2.23.

EXERCISE 2.24.

EXERCISE 2.25.

EXERCISE 2.26.

EXERCISE 2.27.

Bonus exercise.

## CHAPTER 3

### Product operations

**3a.**

**3b.**

**3c.**

**3d.**

**3e. Exercises**

Exercises:

EXERCISE 3.1.

EXERCISE 3.2.

EXERCISE 3.3.

EXERCISE 3.4.

EXERCISE 3.5.

EXERCISE 3.6.

EXERCISE 3.7.

EXERCISE 3.8.

Bonus exercise.



## CHAPTER 4

### Small graphs

4a.

4b.

4c.

4d.

4e. Exercises

Exercises:

EXERCISE 4.1.

EXERCISE 4.2.

EXERCISE 4.3.

EXERCISE 4.4.

EXERCISE 4.5.

EXERCISE 4.6.

EXERCISE 4.7.

EXERCISE 4.8.

Bonus exercise.



## Part II

# Symmetry groups

*At the age of thirty-seven  
She realised she'd never ride  
Through Paris in a sports car  
With the warm wind in her hair*



## CHAPTER 5

### Symmetry groups

5a.

5b.

5c.

5d.

#### 5e. Exercises

Exercises:

EXERCISE 5.1.

EXERCISE 5.2.

EXERCISE 5.3.

EXERCISE 5.4.

EXERCISE 5.5.

EXERCISE 5.6.

EXERCISE 5.7.

EXERCISE 5.8.

Bonus exercise.



CHAPTER 6

**Graph symmetries**

**6a.**

**6b.**

**6c.**

**6d.**

**6e. Exercises**

Exercises:

EXERCISE 6.1.

EXERCISE 6.2.

EXERCISE 6.3.

EXERCISE 6.4.

EXERCISE 6.5.

EXERCISE 6.6.

EXERCISE 6.7.

EXERCISE 6.8.

Bonus exercise.



## CHAPTER 7

### Quantum reflections

7a.

7b.

7c.

7d.

7e. Exercises

Exercises:

EXERCISE 7.1.

EXERCISE 7.2.

EXERCISE 7.3.

EXERCISE 7.4.

EXERCISE 7.5.

EXERCISE 7.6.

EXERCISE 7.7.

EXERCISE 7.8.

Bonus exercise.



CHAPTER 8

**Planar algebras**

**8a.**

**8b.**

**8c.**

**8d.**

**8e. Exercises**

Exercises:

EXERCISE 8.1.

EXERCISE 8.2.

EXERCISE 8.3.

EXERCISE 8.4.

EXERCISE 8.5.

EXERCISE 8.6.

EXERCISE 8.7.

EXERCISE 8.8.

Bonus exercise.





## Part III

# Analytic aspects

*And Michelle, what will she do  
Without you, Lady Madeleine  
And I walk down the avenue  
And I'm missing you, Lady Madeleine*

CHAPTER 9

Counting questions

9a.

9b.

9c.

9d.

9e. Exercises

Exercises:

EXERCISE 9.1.

EXERCISE 9.2.

EXERCISE 9.3.

EXERCISE 9.4.

EXERCISE 9.5.

EXERCISE 9.6.

EXERCISE 9.7.

EXERCISE 9.8.

Bonus exercise.



CHAPTER 10

**Random walks**

**10a.**

**10b.**

**10c.**

**10d.**

**10e. Exercises**

Exercises:

EXERCISE 10.1.

EXERCISE 10.2.

EXERCISE 10.3.

EXERCISE 10.4.

EXERCISE 10.5.

EXERCISE 10.6.

EXERCISE 10.7.

EXERCISE 10.8.

Bonus exercise.



CHAPTER 11

**Random graphs**

**11a.**

**11b.**

**11c.**

**11d.**

**11e. Exercises**

Exercises:

EXERCISE 11.1.

EXERCISE 11.2.

EXERCISE 11.3.

EXERCISE 11.4.

EXERCISE 11.5.

EXERCISE 11.6.

EXERCISE 11.7.

EXERCISE 11.8.

Bonus exercise.





## CHAPTER 12

### Topological aspects

**12a.**

**12b.**

**12c.**

**12d.**

**12e. Exercises**

Exercises:

EXERCISE 12.1.

EXERCISE 12.2.

EXERCISE 12.3.

EXERCISE 12.4.

EXERCISE 12.5.

EXERCISE 12.6.

EXERCISE 12.7.

EXERCISE 12.8.

Bonus exercise.



## Part IV

# Quantum physics

*As soon as you're born, they make you feel small  
By giving you no time instead of it all  
Till the pain is so big you feel nothing at all  
A working class hero is something to be*

CHAPTER 13

**Quantum information**

**13a.**

**13b.**

**13c.**

**13d.**

**13e. Exercises**

Exercises:

EXERCISE 13.1.

EXERCISE 13.2.

EXERCISE 13.3.

EXERCISE 13.4.

EXERCISE 13.5.

EXERCISE 13.6.

EXERCISE 13.7.

EXERCISE 13.8.

Bonus exercise.



CHAPTER 14

**Games and graphs**

14a.

14b.

14c.

14d.

14e. Exercises

Exercises:

EXERCISE 14.1.

EXERCISE 14.2.

EXERCISE 14.3.

EXERCISE 14.4.

EXERCISE 14.5.

EXERCISE 14.6.

EXERCISE 14.7.

EXERCISE 14.8.

Bonus exercise.





CHAPTER 15

**Statistical mechanics**

**15a.**

**15b.**

**15c.**

**15d.**

**15e. Exercises**

Exercises:

EXERCISE 15.1.

EXERCISE 15.2.

EXERCISE 15.3.

EXERCISE 15.4.

EXERCISE 15.5.

EXERCISE 15.6.

EXERCISE 15.7.

EXERCISE 15.8.

Bonus exercise.



CHAPTER 16

**Quantum mechanics**

**16a.**

**16b.**

**16c.**

**16d.**

**16e. Exercises**

Congratulations for having read this book, and no exercises for this final chapter.



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