QUANTUM MECHANICS IN SIMPLE MATRIX FORM

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This book is dedicated
with gratitude and best wishes to

HOWARD G. HANSON

on the occasion of his retirement
after 33 years as
head of the physics department
at the University of Minnesota, Duluth,
where I have learned much
from his teaching and his example.

PREFACE

This book is both very modest and very ambitious. The extent of its subject is modest. It is not a complete book of quantum physics. It treats only the mathematical language of quantum mechanics, the theoretical structure, and that only from the matrix point of view. Other books and sources have to be used along with it to get a full account of either quantum mechanics including wave mechanics or the experiments that reveal the phenomena quantum mechanics describes.

The book is ambitious in making basic quantum mechanics accessible with minimum mathematics. It avoids the mathematics of Hilbert space, Hermitian and unitary matrices, eigenvalues and eigenvectors, and the like. There are no state vectors or wave functions at all. There are no differential equations. The book does not even use calculus or trigonometry. It assumes only basic algebra.

The emphasis is on the matrices representing physical quantities. States are described simply by mean values of physical quantities or equivalently by probabilities for different possible values. This requires using the algebra of matrices and complex numbers together with probabilities and mean values. These bits of mathematics are introduced at the beginning and then used over and over.

I was surprised to find how much can be done this way, with one hand tied. It is not only possible; for many things it is easier or better. For example, calculating correlations of two spins is easier without state vectors. The absence of a continuous range of possible values for angular momentum or oscillator energy comes out more clearly than in standard methods.

Much of this is original. I found new ways to do things. I hope these will be interesting to anyone who teaches quantum mechanics at any level. I use some of them in my graduate course.

This approach reveals the essential simplicity of quantum mechanics by focusing on the bare skeleton and working only with the key elements of the mathematical structure.

The book grew out of a course I teach for college students not majoring in physics. I also use it in a summer program for gifted high-school students. It can be used in different ways by people in various situations. For anyone studying quantum mechanics, it offers an alternative point of view that I hope will be refreshing. It is designed to give the simplest presentation of the basic topics it covers. I think most people who read *Scientific American* can read this book. It can be read along with broader and more descriptive accounts to learn about the new concepts of the physical world at the basis of quantum mechanics. They are interesting to people outside physics but they are not well known and understood because a complete course in quantum mechanics requires sophisticated mathematics. This book offers an opportunity to actually learn some quantum mechanics, do some problems, and use part of the quantum language, without extensive mathematical preparation. The algebra of complex numbers and matrices is fairly simple and rather fun. The book contains over 100 problems. It also contains references to broader descriptive material.

Presenting quantum mechanics entirely in terms of matrices is not a new idea. Matrix mechanics existed more than half a year before wave mechanics. Born wrote a book on quantum mechanics from the point of view of matrix mechanics alone. It was demolished in a review by Pauli. No single method is sufficient for physicists. They should learn all the different ways of doing quantum mechanics.

Here is one easy way to look rather deeply into quantum mechanics.

THOMAS F. JORDAN

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T. F. J.

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SUMMARY

Quantum mechanics is a fundamental language of physics. It is used to describe things on a small scale of size where quantities comparable to Planck's constant are important. It represents knowledge gained from many experiments that reveal properties of atoms and atomic particles that are different from what we know in everyday life. Therefore the language is different.

It is a mathematical language. Its character is determined largely by the mathematics that is used. Imaginary and complex numbers are widely used. Physical quantities such as position coordinates, velocities, momenta, angular momenta, and energies are represented by matrices. The algebra of matrices is different from that of numbers because matrices do not generally commute; the product AB of two matrices A and B may be different from BA.

A quantity may have a definite value for a particular state of the physical system or object being described, but for any state there are quantities that do not have definite values. For example, if a position coordinate has a definite value, the momentum in the same direction does not. If a quantity does not have a definite value for a particular state, there are probabilities for finding different possible values, and there is a mean value corresponding to these probabilities. Every quantity has a mean value for each state. The basic rules of quantum mechanics can be stated very simply in terms of these mean values and the matrices that represent physical quantities. They are mostly rules that are natural to follow in using probabilities. Yet we can calculate quite a bit from them without assuming much more.

The simplest example is a spin and magnetic moment described by Pauli matrices. From the multiplication rules for these matrices, and the basic rules of quantum mechanics, we deduce that there are only two possible values μ and $-\mu$ for the projection of the magnetic moment in a given direction. We also deduce that if a projection in one direction has a definite value, a projection in another direction does not; for a projection in a perpendicular direction, there are equal probabilities $\frac{1}{2}$ for the two possible values. A definite value for a projection in one direction is all we can know. It is all that can be measured. From it we can calculate mean values and probabilities for the projections in other directions.

This example is particularly simple because it involves only 2×2 matrices. We study it thoroughly before we consider systems described by bigger matrices. We determine which matrices represent physical quantities related to the spin and magnetic moment, which represent real quantities, and which non-negative real quantities. We investigate their possible values, mean values, and probabilities. We find which real quantities can have definite values together for the same state; they are represented by matrices that commute. All this serves as a model for general rules of quantum mechanics that we use later.

We consider two spins and the corresponding magnetic moments for two particles. We compute mean values of their products for a state where the total spin is zero. From these we compute probabilities for different pairs of values for projections of the two magnetic moments in various directions.

These quantities are measured in experiments. There are differing predictions of what these experiments should find. One is the result of the calculations using quantum mechanics. The other comes from arguments about objective reality and causality that appear to be good common sense. They grew out of Einstein's criticism of quantum mechanics. They lead to predictions called Bell inequalities. We consider one argument that shows quantum mechanics is inconsistent with simple ideas about reality and causality. We also consider an example of a Bell inequality that conflicts with a result of our calculations in quantum mechanics. Experiments agree with quantum mechanics and not with the other predictions. This is a test of quantum mechanics in an area where there was some doubt. It also shows there is something wrong with the common sense about reality and causality that disagrees with quantum mechanics.

The multiplication rules for the Pauli matrices are the key to all our calculations for spins and magnetic moments. The other quantities we consider are position coordinates and momenta of particles and quantities made from them, such as angular momentum and energy. For these the key equations are the commutation relations of the position and momentum matrices.

These commutation relations imply Heisenberg's uncertainty relation. The product of the uncertainties for position and momentum in the same direction cannot be smaller than Planck's constant divided by 4π. We obtain this as a particular case of an uncertainty relation for any matrices that do not commute. We show that the latter follows from the general rules of quantum mechanics.

We consider the energy of an oscillator, a particle that oscillates back and forth along a line. The energy is quantized; it can have only certain discrete values; there is no continuous range of possible values. We see this by looking at a matrix used to represent the energy. We also show that it follows from the formula for the energy in terms of position and momentum and the commutation relation of the position and momentum matrices. This quantization applies to the energy of oscillation of atoms in a molecule. The energy in an atom also is quantized, as described by the Bohr model. That is related to quantization of the orbital angular momentum.

Matrices that represent angular momentum satisfy characteristic commutation relations. Since orbital angular momentum is made from position and momentum, the commutation relations of the position and momentum matrices imply commutation relations for the matrices representing orbital angular momentum. The same commutation relations hold for the spin angular momentum described by Pauli matrices. We show that these commutation relations determine the values angular momentum can have. It is quantized; it can have only certain discrete values; there is no continuous range of possible values. This quantization applies to the energy of rotational motion of atoms in a molecule, which can be expressed in terms of the orbital angular momentum.

We find the possible values for the energy in a hydrogen atom. We use Pauli's method, which reduces the problem to one that is easily solved with the mathematics of angular momentum. We see how different states with the same energy correspond to different values of quantities that can be measured together with the energy.

Quantum mechanics makes a distinction between a physical quantity and its values. Every quantity is represented by a matrix. For each state, some quantities have definite values and others do not. Equations relating different quantities are written in terms of matrices rather than values. This makes a difference.

For example, position and momentum are not quantized. Each has a continuous range of possible values. We can see this from Heisenberg's uncertainty relation. The oscillator energy is just a combination of the squares of the position and momentum. Yet it is quantized. It has no continuous range of possible values. This can happen because the formula for the energy in terms of position and momentum is written in terms of matrices. It could not happen if the formula were written in terms of values.

There are two kinds of equations that relate matrices representing physical quantities. The formulas for energy and orbital angular momentum in terms of position and momentum are examples of one kind. As relations between physical quantities, these equations would be the same without quantum mechanics. The only difference is that in quantum mechanics they are written in terms of matrices.

Examples of the other kind are the commutation relations for position and momentum and for angular momentum. They would make no sense at all without quantum mechanics because they would make no sense if they were written in terms of values rather than matrices. There were no equations like these before quantum mechanics. They are completely new.

To understand the meaning of these new equations, we consider the way physical quantities change when the space and time coordinates change and the way different changes are related. The matrices are used two different ways. They represent the quantities that describe a particular physical system at a given time. They are also used as multipliers to change the matrices that represent physical quantities to describe the system at another time, or at a different location in space, or rotated to a different orientation in space, or moving at a different velocity. This is where the new equations come in.

All these changes correspond to changes of space and time coordinates. They relate descriptions of the same system by observers who use different coordinates. Changes of coordinates can be multiplied. The product of two changes is defined simply as the result of making first one and then the other. Each change of coordinates is represented by a matrix that is used as a multiplier to change the matrices representing physical quantities. A product of matrices that represent changes of coordinates represents the product of the changes of coordinates.

Products of Pauli matrices correspond to products of 180° rotations. The matrices that represent angular momentum are also used to construct the matrices that represent small rotations. The commutation relations that are characteristic of matrices representing angular momentum correspond to multiplication of rotations. The matrices that represent momentum are used to construct the matrices that represent changes of location in space. The commutation relations of position and momentum matrices correspond to the way position coordinates are changed by changes of space location. In the end, when we consider all the different changes of coordinates, we can deduce almost all the commutation relations.

1 A STRANGE EQUATION

Quantum mechanics is the new language physicists use to describe the things the world is made of and how they interact. It is the basic language of atomic, molecular, solid-state, nuclear, and particle physics. Once found, it was developed quickly, then extended and applied with continuing success as each new area of physics grew. It emerged after a quarter century of work in atomic physics in which experiments revealed properties of the atomic world that could not be understood with the existing theories and led physicists into new ways of thinking.

The first steps toward the new language were taken in 1925 by Werner Heisenberg, then Max Born and Pascual Jordan, those three in collaboration, and Paul Dirac. Born was one of the first people to appreciate what was happening. He expected a new mathematical language, a "quantum mechanics," would be needed for atomic physics, and he had the mathematical knowledge to develop it [1–3]. At 42, Born was an established physicist, a professor at Göttingen. Heisenberg, who was 23, had finished his doctoral studies with Arnold Sommerfeld at Munich and had come to Göttingen to work as Born's assistant. Here is part of Born's recollections.‡

> In Göttingen we also took part in the attempts to distill the unknown mechanics of the atom out of the experimental results. The logical difficulty became ever more acute. ... The art of guessing correct formulas ... was brought to considerable perfection. ...
>
> This period was brought to a sudden end by Heisenberg.... He ... replaced guesswork by a mathematical rule. ... Heisenberg banished the picture of electron orbits with definite radii and periods of rotation, because these quantities are not observable; he demanded that the theory should be built up by means of quadratic arrays ... of transition probabilities.... To me the

‡From Ref. 4. © The Nobel Foundation, 1955.

> decisive part in his work is the requirement that one must find a rule whereby from a given array... the array for the square... may be found (or, in general, the multiplication law of such arrays).
>
> By consideration of ...examples...he found this rule.... This was in the summer of 1925. Heisenberg... took leave of absence... and handed over his paper to me for publication....
>
> Heisenberg's rule of multiplication left me no peace, and after a week of intensive thought and trial, I suddenly remembered an algebraic theory.... Such quadratic arrays are quite familiar to mathematicians and are called matrices, in association with a definite rule of multiplication. I applied this rule to Heisenberg's quantum condition and found that it agreed for the diagonal elements. It was easy to guess what the remaining elements must be, namely, null; and immediately there stood before me the strange formula
>
> $$QP - PQ = \frac{ih}{2\pi}.$$

This is one of the fundamental equations of quantum mechanics. In it Q represents a position coordinate of a particle, P represents the momentum of the particle in the same direction, and i and h are fixed numbers. For an electron in a hydrogen atom, typical values for Q and P are 5×10^{-9} cm and 2×10^{-19} g · cm/s. These are small but otherwise ordinary physical quantities.

Then shouldn't QP be the same as PQ? This equation says they are not the same. That is indeed strange. The number h, which is called Planck's constant, is

$$h \simeq 6.626 \times 10^{-27} \text{ g} \cdot \text{cm}^2/\text{s}.$$

That is very small, so the equation says the difference between QP and PQ is small, but not zero.

There is something else that is strange in this equation. The number i has the property that

$$i^2 = -1$$

so taking the square of both sides of the equation gives

$$(QP - PQ)^2 = \frac{-h^2}{4\pi^2}.$$

Isn't the square of any number positive? How can the square of $QP - PQ$ be negative? We see there are some things that have to be learned before all this can be understood. We will consider the question about squares first and then come back to the question of how QP can be different from PQ.

We can also begin to see that the quantum language gives us a new view of the world. We shall find many features of it that differ from everyday experience and even from common sense. They represent an extension of human knowledge to a much smaller scale of size, to atoms and atomic particles. Nothing as small as Planck's constant would ever be noticed in everyday life. Quantum mechanics is one of the most important and interesting accomplishments of science, but it is not part of our common knowledge. It has been used for over half a century but still, for each of us who learns it, it is strange and wonderful.

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3. D. Serwer, "Unmechanischer Zwang: Pauli, Heisenberg, and the Rejection of the Mechanical Atom, 1923–1925," in *Historical Studies in the Physical Sciences*, Vol. 8, edited by R. McCormmach and L. Pyenson. Johns Hopkins University Press, Baltimore, 1977, particularly pp. 194–195.
4. M. Born, *Science* **122**, 675–679 (1955). This is an English translation of Born's Nobel lecture. I have rewritten the equation in the notation we will use here.

2 IMAGINARY NUMBERS

The number i such that

$$i^2 = -1$$

is called an imaginary number. Inventing it did take some thought and imagination.

Consider the familiar numbers. There are positive numbers such as $\frac{1}{6}$, 1, $\frac{4}{3}$, 2, $\sqrt{2} = 1.4142\ldots$, $\pi = 3.1415\ldots$, the number 0, and negative numbers such as $-\frac{1}{6}, -1, -\pi$. Inventing the negative numbers took some imagination too. By -1 we mean the number such that

$$-1 + 1 = 0,$$

$$-1 + 2 = 1,$$

$$-1 + 3 = 2,$$

and so on. The solution of the equation

$$x + 1 = 0$$

is

$$x = -1.$$

If negative numbers were not invented, there would be no solution of this equation.

If the imaginary number i were not invented, there would be no number z that is a solution of the equation

$$z^2 = -1.$$

The positive and negative numbers and zero are all called real numbers. The square of any real number is either zero or positive. It is never negative. For example,

$$(-2)^2 = 4.$$

Therefore i cannot be a real number. It is different from all the real numbers, something new, just as -1 is different from all the positive numbers.

Starting with -1, we can make other negative numbers by multiplying with positive numbers. For example,

$$-1/6 = (1/6)(-1)$$

$$-\pi = \pi(-1).$$

Starting with i, we can make other imaginary numbers by multiplying with real numbers. For example,

$$(1/6)i = (1/6)(i)$$

$$i\sqrt{2} = (\sqrt{2})(i)$$

$$-i = (-1)(i)$$

$$-i\pi = (-\pi)(i).$$

Let y be a real number. Then

$$iy = yi$$

is an imaginary number. Its square is

$$(iy)^2 = i^2y^2 = -y^2,$$

which is negative, or zero if y is zero.

In particular,

$$(-i)^2 = (-1)^2 i^2 = -1,$$

so the equation

$$z^2 = -1$$

has two solutions

$$z = i \quad \text{and} \quad z = -i.$$