

Matrix Mechanics 109

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What the matrix mechanics of WERNER HEISENBERG, MAX BORN, and PASCUAL JORDAN did was to find another way to determine the "quantum conditions" that had been hypothesized by NIELS BOHR, who was following J.W.NICHOLSON'S suggestion that the angular momentum is quantized. These conditions correctly predicted values for Bohr's "stationary states" and "quantum jumps" between energy levels.

Relativity

But they were really just guesses in Bohr's "old quantum theory," validated by perfect agreement with the values of the hydrogen atom's spectral lines, especially the Balmer series of lines whose 1880's formula for term differences first revealed the existence of integer quantum numbers for the energy levels,

 $1/\lambda = R_{_{\rm H}} (1/m^2 - 1/n^2).$

Heisenberg, Born, and Jordan recovered the same quantization of angular momentum that Bohr had used, but we shall see that it showed up for them as a product of non-commuting matrices.

Most important, they discovered a way to *calculate* the *energy levels* in Bohr's atomic model as well as determine ALBERT EINSTEIN'S 1916 transition probabilities between levels in a hydrogen atom. They could explain the different intensities in the resulting spectral lines.

Before matrix mechanics, the energy levels were *empirically* "read off" the term diagrams of spectral lines. Matrix mechanics is a new mathematical *theory* of quantum mechanics. The accuracy of the old quantum theory came from the sharply defined spectral lines, with wavelengths measurable to six significant figures.

The new quantum theory did not try to interpret or *visualize* what is going on in transitions. Indeed, it strongly discouraged any visualizations. It even denied the existence of electron orbits, a central concept in the Rutherford-Bohr-Sommerfeld atom.

Heisenberg had worked with HENDRIK A. KRAMERS at Bohr's Institute for Physics in Copenhagen to analyze electronic orbits as Fourier series. Kramers had hoped to identify the higher harmonic Chapter 17

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frequencies in the series expansion of orbital frequencies with those of electronic transitions, but Kramer's predictions only worked for large quantum numbers where Bohr's correspondence principle applies.

Kramers' work began with estimates of what were called "dispersion laws" by RUDOLF LADENBERG. The work culminated in the Kramers-Heisenberg dispersion formula in 1925. Based on Bohr's correspondence principle, these led to accurate estimates of the intensities of spectral lines in the hydrogen atom for high quantum numbers. But the assumed orbital frequencies for low quantum numbers did not agree with observations.

Until Heisenberg in 1925, most of the work in the "old quantum theory" focused on *models* of elementary particles. For example, electrons were visualized as going around ERNEST RUTHERFORD's nucleus in orbits, like planets circling the sun. ARNOLD SOMMERFELD extended the Bohr analogy to include Keplerian elliptical orbits with differing angular momentum.

Heisenberg's great breakthrough was to declare that his theory is based entirely on "observable" quantities like the intensities and frequencies of the visible spectral lines.

The attempts by Kramers to predict observed spectral lines as higher harmonics in a Fourier analysis of the *assumed* electronic orbit frequencies ended in failure. But the methods he had developed with Heisenberg's help were adapted by Heisenberg to a Fourier analysis of the *observed* spectral line frequencies. Heisenberg assumed they originate in virtual oscillators like the simple harmonic motion of a vibrating string pinned at the ends or the more complex anharmonic oscillator.

As Kramers had done, Heisenberg identified line intensities with the square of the amplitude of vibrations, which was the classical expression for an oscillating electron. But now Heisenberg's major insight was to calculate values for the position and momentum of the particle using two states rather than one, the initial and final stationary states or energy levels, which we suggested in the chapter on the Bohr atom could simply be "read off" the empirical term diagrams.

Heisenberg's requirement for two states led to an arrangement of transitions in a two-dimensional square array. One dimension was the initial states, the other the final. The array element for i=3 and f=2 represents the transition from level 3 to level 2 with the emission of a light quantum.

When his mentor MAX BORN looked at Heisenberg's draft paper in July of 1925, he recognized the square arrays as *matrices*, a powerful mathematical tool with some unusual properties that played a decisive role in the new quantum mechanics.

Born and his assistant Pascual Jordan submitted a paper within weeks about the strange "non-commuting" of some dynamical variables in quantum mechanics. Normally the order of multiplication makes no difference, ab = ba. But the matrices for the position and momentum operators x and p exhibit what was to become the new "quantum condition," a defining characteristic of the new quantum mechanics.

As Born describes the array,

If we start from the frequencies,

$$v_{nm} = E_n/h - E_m/h,$$

it is a natural suggestion that we arrange them in a square array

| $v_{11} =$ | v_{12} | v_{13} | ••• |
|-------------|-------------|------------------------|-----|
| v_{21} | $v_{22} =$ | <i>V</i> ₂₃ | ••• |
| $v_{_{31}}$ | $v_{_{23}}$ | $v_{33} =$ | ••• |
| | | | |

We can proceed to define the product of two such arrays. The multiplication rule, which Heisenberg deduced solely from experimental facts, runs:

$$(a_{nm})(b_{nm}) = (\Sigma_k a_{nk} b_{km}).^1$$

The central idea of matrix mechanics is that every physical magnitude has such a matrix, including the co-ordinate position and the momentum. However, the product of momentum and position is no longer commutative as in classical mechanics, where the order of multiplication does not matter.

 $p_k q_k = q_k p_k$. Instead, Heisenberg found that

$$p_k q_k - q_k p_k = h/2\pi i.$$

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It is this purely mathematical non-commutation property that is the "quantum condition" for the new quantum mechanics, especially for Paul Dirac, see chapter 19.

But notice that Heisenberg's product of momentum and position has the dimensions of angular momentum. So we are back to Planck's original fortuitive but most insightful guess, and can now add to the answer to our opening question "what is quantized?" This Heisenberg-Born-Jordan discovery that the product of noncommuting quantities p and q leads directly to Planck's constant h, his "quantum" of action, gives us a great insight into what is going on in quantum reality.

It is always angular momentum or spin that is quantized, just as Nicholson had suggested to Bohr, including the dimensionless *isospin* of the neutrons and protons and other sub-elementary particles, which obey the same mathematics as spin and orbital angular momentum for electrons.

And it is the possible projections of the spin or angular momentum onto any preferred directions, such as an external field, that determines possible quantum states. The field is the average over all the dipole and quadrupole moments of other nearby spinning particles.

Heisenberg on Einstein's Light Quanta

Although his matrix mechanics confirmed discrete states and "quantum jumps" of electrons between the energy levels, with emission or absorption of radiation, Heisenberg did not yet accept today's standard textbook view that the radiation is also discrete and in the form of Einstein's spatially localized light quanta, which had been renamed "photons" by American chemist GILBERT LEWIS in late 1926.

Heisenberg must have known that Einstein had introduced probability and causality into physics in his 1916 work on the emission and absorption of light quanta, with his explanation of transition probabilities and prediction of stimulated emission.

But Heisenberg gives little credit to Einstein. In his letters to Einstein, he says that Einstein's work is relevant to his, but does not follow through on exactly how it is relevant. And as late as the Spring of 1926, perhaps following Niels Bohr, he is not convinced of the reality of light quanta. "Whether or not I should believe in light quanta, I cannot say at this stage," he said. After Heisenberg's 1926 talk on matrix mechanics at the University of Berlin, Einstein invited him to take a walk and discuss some basic questions.

We only have Heisenberg's version of this conversation, but it is worth quoting at length to show how little the founders appreciated Einstein's work over the previous two decades on the fundamental concepts of quantum mechanics.:

I apparently managed to arouse Einstein's interest, for he invited me to walk home with him so that we might discuss the new ideas at greater length. On the way, he asked about my studies and previous research. As soon as we were indoors, he opened the conversation with a question that bore on the philosophical background of my recent work. "What you have told us sounds extremely strange. You assume the existence of electrons inside the atom, and you are probably quite right to do so. But you refuse to consider their orbits, even though we can observe electron tracks in a cloud chamber. I should very much like to hear more about your reasons for making such strange assumptions."

"We cannot observe electron orbits inside the atom," I must have replied, "but the radiation which an atom emits during discharges enables us to deduce the frequencies and corresponding amplitudes of its electrons. After all, even in the older physics wave numbers and amplitudes could be considered substitutes for electron orbits. Now, since a good theory must be based on directly observable magnitudes, I thought it more fitting to restrict myself to these, treating them, as it were, as representatives of the electron orbits."

"But you don't seriously believe," Einstein protested, "that none but observable magnitudes must go into a physical theory?"

"Isn't that precisely what you have done with relativity?" I asked in some surprise. "After all, you did stress the fact that it is impermissible to speak of absolute time, simply because absolute time cannot be observed; that only clock readings, be it in the moving reference system or the system at rest, are relevant to the determination of time."

"Possibly I did use this kind of reasoning," Einstein admitted, "but it is nonsense all the same. Perhaps I could put it more diplomatically by saying that it may be heuristically useful to keep in mind what one has actually observed. But on principle, it is quite wrong to try founding a theory on observable magnitudes alone. In reality the very opposite happens. It is the theory which decides what we can observe.

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You must appreciate that observation is a very complicated process. The phenomenon under observation produces certain events in our measuring apparatus. As a result, further processes take place in the apparatus, which eventually and by complicated paths produce sense impressions and help us to fix the effects in our consciousness. Along this whole path - from the phenomenon to its fixation in our consciousness - we must be able to tell how nature functions, must know the natural laws at least in practical terms, before we can claim to have observed anything at all. Only theory, that is, knowledge of natural laws, enables us to deduce the underlying phenomena from our sense impressions. When we claim that we can observe something new, we ought really to be saying that, although we are about to formulate new natural laws that do not agree with the old ones, we nevertheless assume that the existing laws — covering the whole path from the phenomenon to our consciousness-function in such a way that we can rely upon them and hence speak of 'observations' ...

"We shall talk about it again in a few years' time. But perhaps I may put another question to you. Quantum theory as you have expounded it in your lecture has two distinct faces. On the one hand, as Bohr himself has rightly stressed, it explains the stability of the atom; it causes the same forms to reappear time and again. On the other hand, it explains that strange discontinuity or inconstancy of nature which we observe quite clearly when we watch flashes of light on a scintillation screen. These two aspects are obviously connected. In your quantum mechanics you will have to take both into account, for instance when you speak of the emission of light by atoms. You can calculate the discrete energy values of the stationary states. Your theory can thus account for the stability of certain forms that cannot merge continuously into one another, but must differ by finite amounts and seem capable of permanent re-formation. But what happens during the emission of light?

"As you know, I suggested that, when an atom drops suddenly from one stationary energy value to the next, it emits the energy difference as an energy packet, a so-called light quantum. In that case, we have a particularly clear example of discontinuity. Do you think that my conception is correct? Or can you describe the transition from one stationary state to another in a more precise way?"

In my reply, I must have said something like this: "Bohr has taught me that one cannot describe this process by means of the traditional concepts, i.e., as a process in time and space. With that, of course, we have said very little, no more, in fact, than that we do not know. Whether or not I should believe in light quanta, I cannot say at this stage. Radiation quite obviously involves the discontinuous elements to which you refer as light quanta. On the other hand, there is a continuous element, which appears, for instance, in interference phenomena, and which is much more simply described by the wave theory of light. But you are of course quite right to ask whether quantum mechanics has anything new to say on these terribly difficult problems. I believe that we may at least hope that it will one day.

"I could, for instance, imagine that we should obtain an interesting answer if we considered the energy fluctuations of an atom during reactions with other atoms or with the radiation field. If the energy should change discontinuously, as we expect from your theory of light quanta, then the fluctuation, or, in more precise mathematical terms, the mean square fluctuation, would be greater than if the energy changed continuously. I am inclined to believe that quantum mechanics would lead to the greater value, and so establish the discontinuity. On the other hand, the continuous element, which appears in interference experiments, must also be taken into account. Perhaps one must imagine the transitions from one stationary state to the next as so many fade-outs in a film. The change is not sudden—one picture gradually fades while the next comes into focus so that, for a time, both pictures become confused and one does not know which is which. Similarly, there may well be an intermediate state in which we cannot tell whether an atom is in the upper or the lower state."

"You are moving on very thin ice," Einstein warned me. "For you are suddenly speaking of what we know about nature and no longer about what nature really does. In science we ought to be concerned solely with what nature does. It might very well be that you and I know quite different things about nature. But who would be interested in that? Perhaps you and I alone. To everyone else it is a matter of complete indifference. In other words, if your theory is right, you will have to tell me sooner or later what the atom does when it passes from one stationary state to the next"

"Perhaps," I may have answered. "But it seems to me that you are using language a little too strictly. Still, I do admit that everything that I might now say may sound like a cheap excuse. So let's wait and see how atomic theory develops."

Einstein gave me a skeptical look. "How can you really have so much faith in your theory when so many crucial problems remain completely unsolved?"²

Heisenberg (with Bohr) "cannot say at this stage" (1926) whether or not they can "believe in light quanta." Nor do they understand at all Einstein's hope of understanding "objective reality," what nature really does and not just what we can say about it.

² Physics and Beyond, p. 67