Heisenberg's Invention of Matrices

Pradeep Kumar

Richard Feynman once said: "nobody understands quantum mechanics". Still, those who devised it are perhaps the ones closest to understanding their creation. It suggests that whenever the weirdness of quantum mechanics haunts you, it is better to go back to its creators in terms of their original publications. In the present article, the author has tried to seek help from Heisenberg's 1925 paper, in order to reduce the weirdness of going from classical observables to quantum operators.

Pradeep Kumar works as Assistant Professor at the Department of Chemistry, Malaviya National Institute of Technology, Jaipur. He is working in the field of electronic structure calculation, quantum dynamics, and their applications in atmospheric science and spectroscopy.

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It is well known that quantum mechanics was formulated in two different mathematical forms, one of which is known as 'matrix mechanics' and the other as 'wave mechanics'. Initially, there was a divided opinion about which of these formulations represent a more appropriate approach for quantum mechanics. A famous anecdote involving the tense debate between Schrödinger and Heisenberg in Munich during Schrödinger's talk illustrates the differences between these two schools of thoughts (*Box* 1). However, it was soon shown by none other than Schrödinger himself that these two formulations are mathematically equivalent.

Box 1. Schrödinger and Heisenberg – First Encounter

In 1926, Sommerfeld had invited Schrödinger to Munich to deliver two lectures on his wave mechanics. Heisenberg also went there as audience, and the first ever encounter between Schrödinger and Heisenberg took place. During the second lecture, Heisenberg attacked Schrödinger about how matter interacts with radiation through quantum jump. But the audience was in favor of Schrödinger, and in fact the convener (Wein) asked Heisenberg to sit down and be quiet. Later on, he told Heisenberg that his physics, and "with it all such nonsense as quantum jumps" was finished.

Box 2. Hidden Symmetry in Hydrogen Atom

Quantum mechanical state of hydrogen atom is characterized by four quantum numbers – principal (n), azimuthal (l), magnetic (m), and spin (s). But energy depends on only n, and is independent of the other three quantum numbers. This fact is usually explained by invoking the symmetry present in hydrogen atom. The non-dependency of energy on m is attributed to the spherical symmetry of hydrogen atom, but non-dependency on l is not an obvious symmetry. this non-obvious symmetry is known as 'hidden' or 'dynamical' symmetry.

Curiously, modern quantum mechanics books (especially related to chemistry) do not provide detailed descriptions of matrix mechanics. This could be attributed to the fact that Schrödinger wave equation is easier to visualize, while matrix mechanics is far more abstract. Nevertheless, matrix mechanics method sometimes has certain advantages over Schrödinger wave equation method. For example, the hidden or dynamical symmetry[1] of hydrogen atom is not at all obvious using Schrödinger wave equation, whereas without invoking it one cannot solve the hydrogen atom problem using matrix mechanics method (*Box* 2).

[1] See K S Mallesh *etal*., Symmetries and Conservation Laws in Classical and Quantum Mechanics, Vol.16, No.3, pp 254–273,2011.

In the present work, the author does not intend to compare the merits and demerits of these two methods. Instead, the aim is to emphasize certain advantages of matrix mechanics in understanding few basic concepts of quantum mechanics, for example, introduction of quantum operators. By going through matrix mechanics formulation, it becomes apparent that position and momentum should be thought of as mathematical concepts, rather than actual existing observables, like in classical mechanics. Author's personal experience is, by introducing certain basic formulations of matrix mechanics in early classes, students find quantum mechanics less weird. Most of these strange but basic concepts can be understood from Heisenberg's famous 1925 paper, which is considered as the birth of modern quantum mechanics.

Hidden or dynamical symmetry of hydrogen atom is not at all obvious using Schrödinger wave equation.

Box 3. Spectrum of Hydrogen Atom

First good quality spectra of hydrogen atom was recorded in 1853 by Anders Ångström. After 32 years, in 1885, Balmer recognized a pattern in the spectra and gave the Blamer formula: $\lambda = B\frac{m^2}{m^2-2^2}$. Later, Rydberg generalized this formula to: $\frac{1}{\lambda} = \frac{1}{R}(\frac{1}{m^2} - \frac{1}{n^2})$. First successful theoretical explanation of Rydberg formula was given by Bohr–Sommerfeld model, which is now known as 'old quantum mechanics'. Although, the old quantum mechanics was able to explain a lot of facts regarding hydrogen atom spectra, including splitting of spectral lines in presence of electric field (Stark effect), it was still not able to explain quite a few experimental observations such as, splitting of spectral lines in presence of magnetic field (anomalous Zemman effect), presence of hyperfine spectral lines structure and hydrogen atom in presence of crossed electric and magnetic field, etc. Old quantum mechanics was also inadequate to answer why intensity of spectral lines in atomic spectra are different!

Box 4. Hydrogen Atom in Classical Domain

According to classical electrodynamics, orbits of electrons are periodic with periodicity being related to the harmonics of mechanical frequency, i.e., ω, 2ω, etc. As the electron emits electromagnetic radiation, it looses energy. Consequently, radius of orbit becomes smaller, i.e., it exhibits a spiral motion. Although, if the loss of energy is much lesser compared to that of electron's energy, one can neglect the dissipation and electronic motion can be assumed to be periodic.

Heisenberg was trying to understand the spectrum of the hydrogen atom (*Box* 3). Classically, with certain approximations, one expects the spectrum for high energy hydrogen atom to be harmonic (*Box* 4). This fact can be represented by Fourier expansion of position as follows,

By going through matrix mechanics formulation, it becomes apparent that the position and momentum should be thought of as mathematical concepts rather than actual existing observables like in classical mechanics.

$$x(t) = \sum_{n=0}^{\infty} a_n(\omega) \exp(-in\omega t) \ . \quad (1)$$

Here a_n can be related to the intensities of the corresponding harmonics. In the high quantum number limit, the hydrogen atom do exhibit a harmonic spectrum. For example, if we use Rydberg formula: $E_{n_1-n_2} = R * \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$ to calculate transition frequencies from $n_1 = 500$ to $n_2 = 499, 498, 497, 496$, and if $n_{500-499} = \omega_0$

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then other transition frequencies in terms of ω_0 are $2\omega_0$, $3\omega_0$, and $4\omega_0$ respectively.

Heisenberg started with this analogy. He asked the question that if classically, the frequency and intensity of emitted radiations contain information of underlying motion of electron, then why not expect the same from quantum mechanics. Therefore, he thought about the reverse problem and tried to form quantum mechanical position ($x_{qm}(t)$) and momentum from $a_n(\omega)$, and $\exp(-in\omega t)$. Heisenberg started with two observables in case of hydrogen atom,

1. The transition frequency (n_1 *to* n_2).
2. The transition intensities.

It is important to note that quantum mechanics only accounts the observable quantities. For example, as the orbit of the hydrogen atom was not an observable quantity, Heisenberg did not put any attempt to give any physical meaning to it. So, Heisenberg had two pieces of information in his hand – the transition intensities $a(n_1, n_2)$ and transition frequencies $\omega(n_1, n_2)$. It is obvious that these quantities are 2-index objects as compared to their classical counterparts which are typically 1-index objects. Heisenberg realized that the quantum mechanical position should be mathematically related to these 2-index objects, $a(n_1, n_2)\exp(-in\omega(n_1, n_2)t)$. So, he already had the idea that position in quantum mechanics can have a very different meaning, and he was also able to define x_{qm} mathematically. Then he tried to discover the algebra of this object by exploring the multiplication of two x_{qm}. To discover that he again turned to the classical counterpart x^2. Classically,

$$\begin{aligned} x(t)^2 &= \left(\sum_{n=0}^{\infty} a_n(\omega)\exp(-in\omega t)\right)^2 \\ &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} a_n(\omega)a_m(\omega)\exp\{-i(n+m)\omega t\} \\ &= \sum_{p=0}^{\infty} \alpha_p(\omega)\exp(-ip\omega t)\ , \end{aligned} \tag{2}$$

where,

$$\alpha_p(\omega) = \sum_{n=0}^{\infty} a_n(\omega) a_{p-n} \,. \tag{3}$$

So classically, $x(t)^2$ is again a Fourier series, whose coefficients are given by (3). It seems logical at this point to expect that similar to its classical counterpart, quantum mechanically, $x_{qm}(t)^2$ should also be a Fourier series, i.e., $x_{qm}(t)^2 = \sum_{m,n=0}^{\infty} \alpha_{m,n}$ $\exp(-ip\omega(m,n)t)$. But the question is how, the new Fourier coefficients ($a_{m,n}$) and frequencies ($\omega_{m,n}$) are related to the Fourier coefficients corresponding to the expansion of $x(t)$?[2] To explore this relation, Heisenberg again looked towards another experimental observation known as the Ritz combination principle which says,

[2]See how the classical-quantum correspondence plays very important role in the formulation of matrix mechanics.

$$\omega(m,n) = \omega(m,n_1) + \omega(n_1,n). \tag{4}$$

So, the multiplication of two 2-index objects should be in accord with the Ritz principle. Hence the only way 2-index objects can be multiplied should be as follows,

$$a(m,n_1)\exp(-in\omega(m,n_1)t) * a(n_1,n)\exp(-in\omega(n_1,n)t)$$
$$= a(m,n)\exp(-in\omega(m,n)t) \;,$$

and in general,

$$a(m,n)\exp(-in\omega(m,n)t) \;=\; \sum_{n1=1}^{\infty} a(m,n_1)\exp(-in\omega(m,n_1)t)$$
$$\times\, a(n_1,n)\exp(-in\omega(n_1,n)t) \;.$$

Thus, from simply analyzing $x(t)^2$, Heisenberg discovered the algebra of these new 2-index objects. Another very important thing that Heisenberg observed was the non-commutability of different quantum mechanical observables. If we take two observables $x_{qm}(t), y_{qm}(t)$, then contrary to classical mechanics, their product $x_{qm}(t)y_{qm}(t)$ need not be always equal to $y_{qm}(t)x_{qm}(t)$. Now, let us put this algebra in a more modern way so that it becomes familiar. The expression $x_{qm}(t)$ can be arranged in the form of an array,

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$$x_{qm}(t) = \begin{bmatrix} q_{11}, & q_{12}, & q_{13}, & \cdots \\ q_{21}, & q_{22}, & q_{23}, & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix},$$

where $q(m,n) = a(m,n)\exp(-in\omega(m,n)t)$.

Perhaps this rivalry and hatred towards Schrödinger's approach to interpret quantum mechanics, inspired Heisenberg to formulate his most precious contribution to physics – the 'uncertainty principle'.

Now, one can see that if this array is multiplied in Heisenberg's way, then this array is an example of matrix which can be found in any undergraduate mathematics book. It is obvious now that these 2-index objects represent matrices. We know that matrices do not commute always as Heisenberg noticed. Historical fact is, Heisenberg did not know that he was replacing the classical numbers with matrices. It was Heisenberg's mentor Born who recognized that these were actually matrices, and within a few months, with the help of his assistant Pascal Jordan and Heisenberg, he was able to present a more robust formalism of quantum mechanics in terms of these new 2-index objects or matrices. This formulation is known as the 'matrix mechanics method'. The importance of Heisenberg's discovery lies in the replacement of classical numbers by matrices. As a result, the classical observables should be replaced by quantum operators represented by matrices. Another corollary was the translation and reinterpretation of all the classical concepts like position and momentum into this new quantum world. Expectedly, the title of Heisenberg's paper was "A quantum-theoretical re-interpretation of kinematic and mechanical relations". Heisenberg was certain that this new mechanics should be understood in terms of observables only, and that any kind of visualization should have no place. When Schrödinger formulated his wave-mechanics and offered a visualization in terms of his wave-packets, Heisenberg was very upset. He knew that although Schrödinger's formulation was mathematically correct, still there was something wrong in his interpretation. Perhaps this rivalry and hatred toward Schrödinger's approach to interpret quantum mechanics inspired Heisenberg to formulate his most precious contribution to physics – the 'uncertainty principle'[3]. In the next part of this article, the author will explore the Heisenberg commutation relation in the light of his-

[3] See S Lakshmibala, Heisenberg, Matrix Mechanics, and the Uncertainty Principle, Vol.9, No.8, pp.46–56, 2004.

torical Born and Jordan 1925 paper, along with the formulation of uncertainty principle.

Summary

Whenever we proceed from the known into the unknown, we may hope to understand, but we may have to learn at the same time a new meaning of the word 'understanding'.

W Heisenberg

Address for Correspondence
Pradeep Kumar
Department of Chemistry
MNIT Jaipur, Jaipur 302 017,
India.
Email:
pradeep.chy@mnit.ac.in

Suggested Reading

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[4] S Tomonaga, *Quantum Mechanics*, North-Holland, Amsterdam, 1962.