The beginning of Matrix Mechanics

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1 Introduction

The ideas that guided physicist in the early 20th century to decipher the Nature of matter and rediation can be summed up as follows

1. Firstly, M. Planck solves the problem of the radiation of black bodies. He introduces the quanta of energy $E = \hbar\omega$; however, to him it was a mere mathematical trick and no true feature of Nature. Later, A. Einstein takes Planck's relation and elevates it into a true feature of physics. He does this in two cases, first for light (or electromagnetic radiation), now that we call photons, and then for solids, where he quantised the vibrations of ions, thus solving the specific heat problem of solids.

2. Secondly, the idea of virtual or Hertzian oscillators. This idea was introduced by many physicists independently of each other and with different contexts. First by H. Hertz, then by H. Lorentz for his study of dispersion. Also by A. Einstein, R. Ladenburg and J. Slater. To idea of virtual oscillators persists to this day, where we imagine quantum fields (particles) as a collection of virtual oscillators. Without this idea, Quantum Field Theory could not have developed the way it did.

3. Thirdly, the idea of quantising different degrees of momentum. First, N. Bohr introduced the idea of quantising the azimuthal action $p_\theta = n_\theta \hbar$, then A. Sommerfeld refined this idea by generalising to all action variables. Independently, W. Wilson published the same ideas as Sommerfeld. Later, in the now famous Stern-Gerlach experiment, O. Stern and W. Gerlach wanted to measure the polar action quantisation, which was called spatial quantisation, and the idea of spatial quantisation was even refuted by M. Born himself. Later, this Wilson-Sommerfeld quantisation will be a particular interest to W. Heisenberg.

4. Lastly, the importance of discreteness in the quantum world. First, A. Einstein showed that light is a collection of discrete energy packets. Then N. Bohr emphasised that in atoms, energy jumps also occur in discrete amounts, further spreading Einstein's ideas. Then there was the Ritz combination principle discovered by W. Ritz during his efforts to study

the nature of spectral lines. Its most elegant mathematical form was cast by M. Born, who showed that continuous derivatives need to be replaced by discrete differences at the quantum level.

However, all these achievements of Old Quantum Theory were in vain because it was not consistent and it could not explain all processes, especially it was not suitable for the description of dispersion relation. The Lorentz-Lorenz dispersion relation tells us that the refractive index is

$$n = 1 + \frac{e^2 N}{2\varepsilon_0 m} \frac{\omega_0^2 - \omega^2 - i\gamma\omega}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \tag{1}$$

Where N is the number density of electrons. This phenomenon was called the anomalous dispersion, and when Lorentz completed his calculations, this was the classical interpretation of the reason behind the emergence of spectral lines. For many oscillators, this was generalised as

$$n - 1 = \frac{e^2}{2\varepsilon_0 m} \sum_k \frac{N_k}{\omega_k^2 - \omega^2 + i\gamma_k\omega} \tag{2}$$

The summation is introduced because there could be several resonant frequencies. After performing several experiments and measuring electron densities, R. Ladenburg decided to give a quantum mechanical derivation and explanation of the spectral lines. First of all, he used Einstein's A and B coefficients from Einstein's theory of radiation. The equations read

$$\frac{dN_j^{(spe)}}{dt} = -A_{jk}N_j \tag{3}$$

$$\frac{dN_j^{(abs)}}{dt} = B_{kj}N_k\rho(\omega) \tag{4}$$

$$\frac{dN_j^{(ste)}}{dt} = -B_{jk}N_j\rho(\omega) \tag{5}$$

where $\rho(\omega)$ is the energy density. Ladenburg expressed the quantum current as

$$J = \hbar\omega_{jk}(A_{jk}N_j + B_{jk}N_j\rho(\omega)) = -\hbar\omega_{kj}B_{kj}N_k\rho(\omega) \tag{6}$$

Einstein identified the fraction of A and B coefficients as (based on Planck's equation)

$$\frac{A_{jk}}{B_{jk}} = \frac{\hbar\omega_{jk}^3}{\pi^2 c^3} \tag{7}$$

The B coefficents can be related with the probabilities as $p_k B_{kj} = B_{jk}p_j$, thus Ladenburg's quantum current becomes

$$J = N_k \frac{p_j}{p_k} A_{jk} \frac{\pi^2 c^3}{\omega_{jk}^2} \rho(\omega) \tag{8}$$

There are two important things to note about Laudenberg's results: the first is that before the advent of quantum mechanics, physicists did not treat the indices with care, and only after the introduction of matrices by Heisenberg, Born and Jordan did they start to treat them much more carefully. Secondly, the importance of angular frequencies in the result. These oscillators are the ones that we call virtual oscillators (the term was coined by Bohr). This is an important step because this will guide Heisenberg in finding his reinterpretation of Quantum Mechanics. Finally, the index of refraction becomes in Ladenburg's interpretation

$$n - 1 = \frac{e^2 \pi^2 c^3}{2\varepsilon_0 m} \sum_k \frac{p_j}{p_k} A_{jk} \frac{1}{\omega_{jk}^2} \rho(\omega) \frac{N_k}{\omega_{jk}^2 - \omega^2} \tag{9}$$

This formula was further refined by Kramers and Heisenberg, giving us

$$n - 1 = \frac{e^2 \pi^2 c^3}{2\varepsilon_0 m} \left(\sum_{k>j} \frac{p_j}{p_k} A_{jk} \frac{1}{\omega_{jk}^2} \rho(\omega) \frac{N_k}{\omega_{jk}^2 - \omega^2} - \sum_{k<j} \frac{p_j}{p_k} A_{kj} \frac{1}{\omega_{kj}^2} \rho(\omega) \frac{N_k}{\omega_{kj}^2 - \omega^2} \right) \tag{10}$$

However, Kramers' justification initially was not that convincing, and it took him two more articles to give a full mathematical derivation of his formula. The main problem why others criticised Kramers was the introduction of the minus sign in his second term. The derivation relied on Old Quantum Theory and was really long and cumbersome to perform the calculations.

2 Matrix Mechanics

In 1925, Werner Heisenberg took a trip to the island of Helgoland to recover from an illness. In the few days he spent on the island, he reinterpreted quantum mechanics. He had several key ideas, namely

1. Heisenberg sacrificed the idea of the motion of quantum particles, as was the case with old quantum theory. Instead, he said that only observables are important, i.e. the energy jumps in an atom.

2. The usage of virtual oscillators. The motion was considered periodic; hence, the Fourier expansion was used by Heisenberg. Although he replaced the classical indices by new quantum mechanical ones (i.e. he introduced matrices into the Fourier series). This assumption was not that strange since in old quantum theory, Action-Angle variables can only be used if a motion is periodic. However, the way Heisenberg went about it is new.

3. The Sommerfeld-Wilson quantisation rule seemed arbitrary to Heisenberg because the quantum number n was arbitrary. Hence, he took the difference of that equation to eliminate that dependence and thus introduced the quantum canonical commutation relation (its final form is due to Born and Jordan)

4. Finally, the most surprising is that Heisenberg used Newtonian mechanics to describe his motion. Later, this was elevated to the much more elegant Hamiltonian dynamics by Born and Jordan. However, I feel that after learning quantum mechanics in its modern form, we surprisingly find that classical equations of motion dictate how matter and radiation behave on the quantum level.

Following Heisenberg's original paper is quite difficult, and I found that Born and Jordan's paper is more coherent. We will look at the postulates of Matrix mechanics and two examples, the harmonic oscillator solved by Heisenberg and the Hydrogen atom solved by Pauli. Lastly, it will shortly be demonstrated how the de Broglie-Schrödinger wave mechanics reduces to Heisenberg-Born-Jordan matrix mechanics. Finally, it will be discussed why the matrix formulation has fallen out of use, and the wave mechanics stands tall in the calculation of quantum mechanics, and a surprising reemergence of matrices in computer simulations.

In their paper simply titled '*On Quantum Mechanics*', M. Born and P. Jordan came up with the following postulates

Postulate 1. A dynamical system that is described by generalised coordinate $\mathbf{q}$ and canonical momentum $\mathbf{p}$ is to be replaced by matrices. Namely they become

$$\mathbf{q} = q_{nm}e^{i\omega_{nm}t} \tag{11}$$

$$\mathbf{p} = p_{nm}e^{i\omega_{nm}t} \tag{12}$$

where $\omega_{nm} = -\omega_{mn}$ is the angular frequency between transitions of nth and mth state. The amplitud of coordinate and momentum is given by $|q_{nm}|^2 = \sum_m q_{nm}q_{mn}^*$ and $|p_{nm}|^2 = \sum_m p_{nm}p_{mn}^*$ and all matrices to be Hermitian (Hermitian matrices have real eigenvalues, and all phyisically observables have real, positive values).

Postulate 2. All dynamical system with angular frequency ω_{nm} shall satisfy the following combination formula

$$\omega_{ij} + \omega_{jk} + \omega_{ki} = 0 \tag{13}$$

Before postulating this equation was known as the Ritz combination principle. The significance of this rule is that it explains the relations of spectral lines in spectroscopy. For Born and Jordan, the above equation does not imply that

$$\hbar\omega_{nm} = E_n - E_m \tag{14}$$

That is Bohr's frequency condition. To them, it was simply about the physically observable spectral lines and not about the energy. The Bohr frequency condition had to be derived rigorously.

Postulate 3. For a dynamically conserved motion having a Hamiltonian such as

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + \mathbf{V}(\mathbf{q}) \tag{15}$$

Hamilton's equation of motion shall remain true with the appropriate matrix replacements. Hamilton's equations say

$$\dot{\mathbf{q}} = \frac{\partial \mathbf{H}}{\partial \mathbf{p}} \tag{16}$$

$$\dot{\mathbf{p}} = -\frac{\partial \mathbf{H}}{\partial \mathbf{q}} \tag{17}$$

In the interpretation of Heisenberg, Born and Jordan, the problem was not dynamics (the form of equations, Hamilton's equations) but rather kinematics (what is the meaning behind coordinate and momentum).

Postulate 4. The diagonal elements H_{nn} of $\mathbf{H}$ are interpreted as the energies of various states of the system. The equation in it matrix form reads

$$H_{nm} = E_n \delta_{nm} \tag{18}$$

where δ_{nm} is the Kronecker delta. The new idea in this was that calculating the energies of a system is reduced to finding its diagonal elements of the Hamiltonian matrix. In the Old Quantum Theory, it was difficult to say why energy needed to be quantised. It had to be artificially postulated or imposed on the system. However, matrices are naturally quantised, and Bohr's concept of stationary energy state finally had a rigorous mathematical foundation in the new quantum mechanics.

Postulate 5. The elements of $\mathbf{p}$ and $\mathbf{q}$ satisfy the following quantum condition, which has been reformulated as

$$\sum_k p_{nk} q_{km} - q_{nk} p_{km} = \frac{\hbar}{i} \delta_{nm} \tag{19}$$

Or in modern notation, we have the canonical commutation relation, which is

$$[\mathbf{q}, \mathbf{p}] = i\hbar \tag{20}$$

Since this relation is so important and it is one of the main concepts in quantum mechanics, a 'derivation' will be given below.

The derivation of the *Quantum Condition* begins with the Action definition and the Fourier series. Hence we have

$$I = \frac{1}{2\pi} \oint p\, dq = \frac{1}{2\pi} \int_0^{\frac{2\pi}{\omega_0}} p\dot{q}\, dt \tag{21}$$

Expressing the coordinate and momentum in classical Fourier series, we have

$$q = \sum_{k=-\infty}^{\infty} q_k e^{i\omega_k t} \tag{22}$$

$$p = \sum_{k=-\infty}^{\infty} p_k e^{i\omega_k t} \tag{23}$$

where ω_k is equal to $k\omega_0$. Substituting those equations in, we get for the action

$$I = \frac{1}{2\pi} \sum_{k,l=-\infty}^{\infty} \int_0^{\frac{2\pi}{\omega_0}} i\omega_k \, p_l q_k e^{i(\omega_l+\omega_k)t} \, dt \tag{24}$$

$$= \frac{1}{2\pi} \sum_{k,l=-\infty}^{\infty} i\omega_k \, p_l q_k \int_0^{\frac{2\pi}{\omega_0}} e^{i(\omega_l+\omega_k)t} \, dt \tag{25}$$

$$= \frac{i}{2\pi} \sum_{k,l=-\infty}^{\infty} \omega_k \, p_l q_k \int_0^{\frac{2\pi}{\omega_0}} e^{i(l+k)\omega_0 t} \, dt \tag{26}$$

Where in the last line we recognise an integral representation of the Kronecker delta, especially if we do the change of variables $\varphi = \omega_0 t$, the integral simplifies to

$$I = \frac{i}{2\pi} \sum_{k,l=-\infty}^{\infty} k \, p_l q_k \int_0^{2\pi} e^{i(l+k)\varphi} \, d\varphi \tag{27}$$

$$= i \sum_{k,l=-\infty}^{\infty} k \, p_l q_k \delta_{l,-k} \tag{28}$$

$$= i \sum_{k=-\infty}^{\infty} k \, p_{-k} q_k \tag{29}$$

Since, in the eyes of Heisenberg, Born and Jordan, this action was arbitrary, they took its differentiated form, with respect to action, then introduced one of Born's ideas that continuous derivatives are being replaced with discrete [1] Then we have

$$1 = i \sum_{k=-\infty}^{\infty} k \frac{\partial}{\partial I} p_{-k} q_k \tag{30}$$

$$= i \sum_{k=-\infty}^{\infty} k \left(\frac{\partial p_{-k}}{\partial I} q_k + p_{-k} \frac{\partial q_k}{\partial I} \right) \tag{31}$$

$$= i \sum_{k=-\infty}^{\infty} \left(p_{-k} \, k \frac{\partial q_k}{\partial I} - (-k) \frac{\partial p_{-k}}{\partial I} q_k \right) \tag{32}$$

$$= \frac{i}{\hbar} \sum_{k=-\infty}^{\infty} (p_{n,n+k} \, q_{n,n+k} - p_{n,n-k} \, q_{n-k,n}) \tag{33}$$

$$= \frac{i}{\hbar} \sum_{m=-\infty}^{\infty} (p_{n,m} \, q_{m,n} - q_{n,m} \, p_{m,n}) \tag{34}$$

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[1] By Born we have $k\frac{\partial f_{n,k}}{\partial n} \to f_{n+k,n} - f_{n,n-k}$. For the $-k$ case, just replace all the ks with $-k$s in the previous relationship

Where we used the fact that the derivative can be written as a in two different ways because of k and $-k$. Finally, we used Heisenberg's principle of replacing classical indices with quantum indices. Finally, giving us the quantum condition of

$$\frac{\hbar}{i} = \sum_{m=-\infty}^{\infty} (p_{n,m}\, q_{m,n} - q_{n,m}\, p_{m,n}) \tag{35}$$

The main thing to take away from these postulates and in the derivation of the quantum condition is that the dependence of ω_{nm}, p_{nm}, and q_{nm} on the indices n and m should not be arbitrarily imposed, as is the case in Old Quantum Theory but rather to be built in to theory and the way the conjugate variables interact.

The Harmonic oscillator is one of the most important examples in quantum mechanics. Here is how Heisenberg solved it using the newly developed quantum mechanics. The main equations are as follows

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega_0^2\mathbf{q}^2 \tag{36}$$

$$0 = \ddot{\mathbf{q}} + \omega_0^2\mathbf{q}^2 \tag{37}$$

$$i\hbar = [\mathbf{q}, \mathbf{p}] \tag{38}$$

Rewriting them with indices and, using that $p_{nm} = m\dot{q}_{nm} = im\omega_{nm}q_{nm}$, they become

$$H_{nm} = \frac{m}{2}(\omega_{nm}^2 q_{nm}^2 + \omega_0^2 q_{nm}^2) \tag{39}$$

$$0 = (\omega_0^2 - \omega_{nm}^2)q_{nm} \tag{40}$$

$$i\hbar = im(\omega_{nm}|q_{nm}|^2 - \omega_{mn}|q_{mn}|^2) \tag{41}$$

Then further simplifying the calculations with the fact that the angular frequency matrix is antisymmetric $\omega_{nm} = -\omega_{mn}$ we get

$$H_{nm} = m\omega_0^2|q_{nm}|^2 \tag{42}$$

$$\frac{\hbar}{2m} = \omega_{nm}|q_{nm}|^2 = \omega_0|q_{nm}|^2 \tag{43}$$

For some index n, m, we find that there are only two elements in the matrix row that are non-zero (implicit summation is assumed). And if for some index, say $n = 0$, we have that there is only one element that is different from zero, that is to say that Heisenberg lived with the assumption of there exist a ground state to which there exist no lower energy levels, which will give us

$$\frac{\hbar}{2m\omega_0} = |q_{0m}|^2 \tag{44}$$

$$E_0 = \frac{\hbar\omega_0}{2} \tag{45}$$

7

In the last equation, there is no implicit summation. The higher-order formula arises from the fact that when we are not in the ground state, there are two non-zero elements in the matrix row, and we can express them recursively, giving us the final formula for the energy of a quantum harmonic oscillator

$$E_n = \hbar\omega_0 \left(n + \frac{1}{2} \right) \tag{46}$$

$$= (2n + 1)E_0 \tag{47}$$

The energy gap between two consecutive levels of a harmonic oscillator is $\Delta E_n = 2E_0$. These results of Heisenberg were later reproduced by M. Born, P. Jordan, and P. A. M. Dirac. Finally, Heisenberg, in his seminal paper, treated the problem of the anharmonic oscillator by applying perturbation theory and building on the result of the harmonic oscillator. A final mathematical remark. Since technically all of these matrices should be infinite times infinite matrices, we have to turncut them at some point. When we apply this turncution we get that the last entry will deviate from the general formula.

The final problem that had to be solved was the problem of the Hydrogen atom. This was solved by W. Pauli by using a clever idea from the Kepler problem, namely the constant of motion named the Laplace-Runge-Lenz vector. In classical mechanics, it takes the form of

$$\mathbf{A} = \mathbf{p} \times \mathbf{L} - \frac{me^2 Z}{4\pi\varepsilon_0} \frac{\mathbf{r}}{r} \tag{48}$$

This equation is valid for any spherically symmetric potentials. That is said for

$$\mathbf{F} = -\frac{k}{r^3}\mathbf{r} \tag{49}$$

For further use it is useful to state the LRL-vector in component form. The equation looks like

$$A_i = \varepsilon_{ijk}p_i L_j - \frac{me^2 Z}{4\pi\varepsilon_0} \frac{q_i}{r} \tag{50}$$

Since due to the equation of Canonical commutation

$$[\mathbf{q}, \mathbf{p}] = i\hbar \tag{51}$$

Pauli had to anti-symmetrize the cross product because coordinate and momentum did not commute with each other anymore. Hence Pauli wrote

$$A_i = \frac{1}{2}(\varepsilon_{ijk}p_i L_j - \varepsilon_{ijk}L_i p_j) - \frac{me^2 Z}{4\pi\varepsilon_0} \frac{q_i}{r} \tag{52}$$

These operators satiesfy the following commutation relations and properties

$$[L_i, L_j] = i\hbar\varepsilon_{ijk}L_k \tag{53}$$

$$[L_i, A_j] = i\hbar\varepsilon_{ijk}A_k \tag{54}$$

$$[A_i, A_j] = -2im\hbar\,H\,\varepsilon_{ijk}A_k \tag{55}$$

$$L_iA_i = A_iL_i = 0 \tag{56}$$

$$A_i^2 = 2mH(L_i^2 + \hbar^2) + \frac{m^2e^4Z^2}{16\pi^2\varepsilon_0^2} \tag{57}$$

where H is the Hamiltonian of the system and is given by

$$H(r, p_r, L^2) = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} - \frac{e^2}{4\pi\varepsilon_0 r} \tag{58}$$

The main importance of the Hamiltonian in the commutation rules, is that according the Heisenberg-Born-Jordan interpretation the diagonal elements of the Hamiltonian will give us the energies. That is

$$H_{nm} = E_n\delta_{nm} \tag{59}$$

What we want next is to independent SO(3) group that commutes with each other. Hence, Pauli defined the following 'ladder' operators

$$I_i = \frac{1}{2}\left(L_i + \frac{i}{\sqrt{2mH}}A_i\right) \tag{60}$$

$$K_i = \frac{1}{2}\left(L_i - \frac{i}{\sqrt{2mH}}A_i\right) \tag{61}$$

And their Commutation relation reads

$$[I_i, I_j] = i\hbar\varepsilon_{ijk}I_k \tag{62}$$

$$[K_i, K_j] = i\hbar\varepsilon_{ijk}K_k \tag{63}$$

$$[I_i, K_j] = 0 \tag{64}$$

In their follow up paper of Heisenberg, Born, and Jordan (physics historians call this paper the 'Dreimännarbeit'), establish the follwoing result for the angular momentum operators

$$L_{z,nm} = l_{z,n}\hbar\delta_{nm} \tag{65}$$

$$L_{nm}^2 = n(n+1)\hbar\delta_{nm} \tag{66}$$

$$\tag{67}$$

Applying these results for the new operators, and rewriting the second property of the LRL-vector, we get

$$\frac{me^4 Z^2}{32\pi^2 \varepsilon_0^2 H} = L_i^2 - \frac{1}{2mH} A_i^2 + \hbar^2 \tag{68}$$

$$-\frac{me^4 Z^2}{32\pi^2 \varepsilon_0^2 H} = 2(I_i^2 + K_i^2) + \hbar^2 \tag{69}$$

$$-\frac{me^4 Z^2}{32\pi^2 \varepsilon_0^2 E_i} = (2i+1)^2 \hbar^2 \tag{70}$$

$$E_i = -\frac{me^4 Z^2}{32\pi^2 \varepsilon_0^2 \hbar^2 (2i+1)^2} \tag{71}$$

$$E_i = -\frac{E_0 Z^2}{(2i+1)^2} \tag{72}$$

The final step is to identify the principal quantum number n, which leads to

$$E_n = -\frac{E_0 Z^2}{n^2} \tag{73}$$

With these calculations, Pauli recovered Bohr's results for the hydrogen atom. I think the brilliance in this approach that we nowadays we do not use is that we used a constant of motion, namely the Laplace-Runge-Lenz vector, which can be directly correlated to the energy of the system. Finally, it is also remarkable that Pauli were able to get this result, since matrices are fine for linear motion such as the harmonic oscillator but it is very awkward to use for non-linear motion such as spherical coordinates. Further more Pauli was also able to study the Zeemann and Stark effect using the newly developed matrix mechanics. To evaulate this electromagnetic phenomena Pauli, lived with the following assumptions such as the proton is infinitely massive and the diamagnetic term can be neglected. Then the interaction Hamiltonian becomes

$$H_{int} = eE_i q_i + \frac{e}{2m} L_i B_i \tag{74}$$

Then substituting in the independent generators of SO(3) algebras I_i and K_i we got

$$H_{int} = \frac{1}{\hbar}\left(-\frac{3a_0 n}{2} E_i + \frac{e\hbar}{2m} B_i\right) I_i + \frac{1}{\hbar}\left(\frac{3a_0 n}{2} E_i + \frac{e\hbar}{2m} B_i\right) K_i \tag{75}$$

where n is the principle quantum number and a_0 is given by

$$a_0 = \frac{4\pi \varepsilon_0 \hbar^2}{me} \tag{76}$$

Then the energy becomes

$$H_{int} = E^+ \frac{n_i^+ I_i}{\hbar} + E^- \frac{n_i^- K_i}{\hbar} \tag{77}$$

10

Where the follwing quantities were defined

$$E^{\pm} = \sqrt{\left(\pm\frac{3a_0 n}{2}E_i + \frac{e\hbar}{2m}B_i\right)^2} \tag{78}$$

$$n^{\pm} = \frac{1}{E^{\pm}}\left(\pm\frac{3a_0 n}{2}E_i + \frac{e\hbar}{2m}B_i\right) \tag{79}$$

Then using the Campbell-Baker-Hausdorf formula and expanding it we get to first order the following correction to the energy of the hydrogen atom in the presence of electric and magnetic fields

$$\Delta E_n^{(1)} = l_z E^{+} + k_z E^{-} \tag{80}$$

where l_z and k_z are the third components of the respective angular momentum matrices.

3 The fall and reemergence of Matrix Mechanics

In the following years after 1925, Heisenberg's matrix interpretation of quantum mechanics got further elaborated by him, Born, Jordan, Pauli and Dirac. However, this transcendental algebra of matrices was new for most physicists and they needed to learn this new mathematics to be able to get the correct result for the theoretical computations. However, in parallel with the development of Matrix Mechanics, L. de Broglie and E. Schrödinger started the development of Wave Mechanics. When they completed their work, matrices were replaced with differential operators and the natural quantisation, discreteness entered in the form of using series expansion to solve the partial differential equations with restrictions on asymptotics. This latter method became more popular since physicists were already used to and familiar with partial differential equations. Furthermore, Schrödinger's work became more popular because it incorporated time dependence and could be easily generalised for more complex problems, then it could be done with matrix mechanics. However, it is important to point out that both formulations of quantum mechanics are equivalent to each other. In the following, I will shortly demonstrate how we can derive the matrix form of the Canonical Commutation relation from its functional cousin.

First of all we are gonna define the position and momentum matrices as the expectation values from wave mechanics.

$$q_{nm} = \int_{\mathbb{R}} \phi_n^*(x)\ x\ \phi_m(x)\,dx \tag{81}$$

$$p_{nm} = \int_{\mathbb{R}} \phi_n^*(x)\left(-i\hbar\frac{d\phi_m}{dx}(x)\right)dx \tag{82}$$

Then we carefully evaluate the matrix products as the series expansions from

the Sturm-Liouville theory

$$p_{nk}q_{km} = \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \frac{d}{dx} \left[\phi_k(x) q_{km} \right] \, dx \tag{83}$$

$$= \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \frac{d}{dx} \left[\phi_k(x) \int_{\mathbb{R}} \phi_k^*(y) \, y \, \phi_m(y) \, dy \right] dx \tag{84}$$

$$= \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \frac{d}{dx} \left[x \, \phi_m(x) \right] dx \tag{85}$$

$$= \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \phi_m(x) dx + \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \, x \, \frac{d\phi_m(x)}{dx} \, dx \tag{86}$$

$$= \frac{\hbar}{i} \delta_{nm} + \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \, x \, \frac{d\phi_m(x)}{dx} \, dx \tag{87}$$

Performing a similar calculation for the other half of the commutation relation we find

$$q_{nk}p_{km} = \int_{\mathbb{R}} \phi_n^*(x) \, x \, \left[\phi_k(x) p_{km} \right] \, dx \tag{88}$$

$$= \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \, x \, \left[\phi_k(x) \int_{\mathbb{R}} \phi_k^*(y) \frac{d\phi_m(y)}{dy} \, dy \right] dx \tag{89}$$

$$= \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \, x \, \left[\frac{d\phi_m(x)}{dx} \right] dx \tag{90}$$

$$= \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \, x \, \frac{d\phi_m(x)}{dx} \, dx \tag{91}$$

Subtracting the two results from each other, we get

$$p_{nk}q_{km} - q_{nk}p_{km} = \frac{\hbar}{i} \delta_{nm} + \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \, x \, \frac{d\phi_m(x)}{dx} \, dx - \frac{\hbar}{i} \int_{\mathbb{R}} \phi_n^*(x) \, x \, \frac{d\phi_m(x)}{dx} \, dx \tag{92}$$

$$= \frac{\hbar}{i} \delta_{nm} \tag{93}$$

Thus, from Schrödinger's theory, we have derived the matrix commutation rules pioneered by Born, Jordan and Heisenberg.

However, matrix mechanics experienced a resurgence with the rise of computers. The need for matrices in computers arises naturally since computers can only compute discrete points on a grid. When we approximate a differential operator with a difference, we actually construct its correct matrix representation.

$$\frac{-\hbar^2}{2m} \nabla^2 \psi \, + \, V\psi = E\psi \tag{94}$$

$$\frac{-\hbar^2}{2m} (\psi_{n+2} - 2\psi_{n+1} + \psi_n) \, + \, V\psi_n = E\psi_n \tag{95}$$

12

As we can constructed a matrix which is multiplied by the follwoing probability vector $\{\psi_{n+2}, \psi_{n+1}, \psi_n\}$, and our task is to find the eigenvalue of the above matrix, just as was the case in Heisenberg's and Born's case. Furthermore, Born developed the probability interpretation and introduced the probability vectors to further expand on Heisenberg's work. This interpretation of Born's still presist to this day determining how we see and imagine our Universe.

References

[1]   H. Goldstein, Ch. Poole, J. Safko: Classical Mechanics Third edition, Addison-Wesley, p. 430-483 & p. 526-558 `https://homepages.dias.ie/ydri/Goldstein.pdf`

[2]   Chung Wen Kao: From Old Quantum Theory to Quantum Mechanics `https://www.phys.sinica.edu.tw/files/20200114_ChungWenKao.pdf`

[3]   Jorge S. Diaz: Quantum Mechanics `https://www.youtube.com/watch?v=gXeAp_lyj9s&list=PL_UV-wQj1lvVxch-RPQIUOHX88eeNGzVH&pp=0gcJCa4EOCosWNin`

[4]   Günter Lydik: Quantum Mechanics in Matrix Form, Springer

[5]   Sander Konijnenberg: Towards quantum mechanics `https://www.youtube.com/watch?v=FFDjTTp7ygM&list=PLG6kLm-LDbaCJhFMH8S7vVj8U_itLoik4`