QUANTUM MECHANICS

James Freericks, Department of Physics
Georgetown University
Work funded by the AFOSR and Georgetown

Modern quantum mechanics started with matrix mechanics in 1925

But, does anyone really know how the original idea worked?

It all started in the summer and fall of 1925 with three critical papers

Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen.

Von **W. Heisenberg** in Göttingen.

(Eingegangen am 29. Juli 1925.)

In der Arbeit soll versucht werden, Grundlagen zu gewinnen für eine quantentheoretische Mechanik, die ausschließlich auf Beziehungen zwischen prinzipiell beobachtbaren Größen basiert ist.

It all started in the summer and fall of 1925 with three critical papers

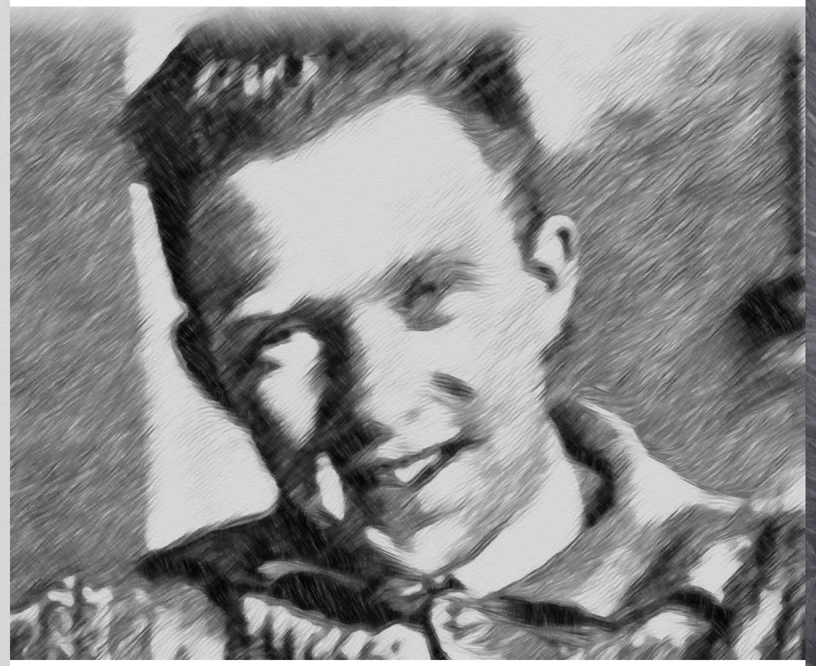
Zur Quantenmechanik.

Von **M. Born** und **P. Jordan** in Göttingen.

(Eingegangen am 27. September 1925.)

Die kürzlich von Heisenberg gegebenen Ansätze werden (zunächst für Systeme von einem Freiheitsgrad) zu einer systematischen Theorie der Quantenmechanik entwickelt. Das mathematische Hilfsmittel ist die Matrizenrechnung. Nachdem diese kurz dargestellt ist, werden die mechanischen Bewegungsgleichungen aus einem Variationsprinzip abgeleitet und der Beweis geführt, daß auf Grund der Heisenbergschen Quantenbedingung der Energiesatz und die Bohrsche Frequenzbedingung aus den mechanischen Gleichungen folgen. Am Beispiel des anharmonischen Oszillators wird die Frage der Eindeutigkeit der Lösung und die Bedeutung der Phasen in den Partialschwingungen erörtert. Den Schluß bildet ein Versuch, die Gesetze des elektromagnetischen Feldes der neuen Theorie einzufügen.

It all started in the summer and fall of 1925 with three critical papers


Zur Quantenmechanik. II.

Von **M. Born, W. Heisenberg** und **P. Jordan** in Göttingen.

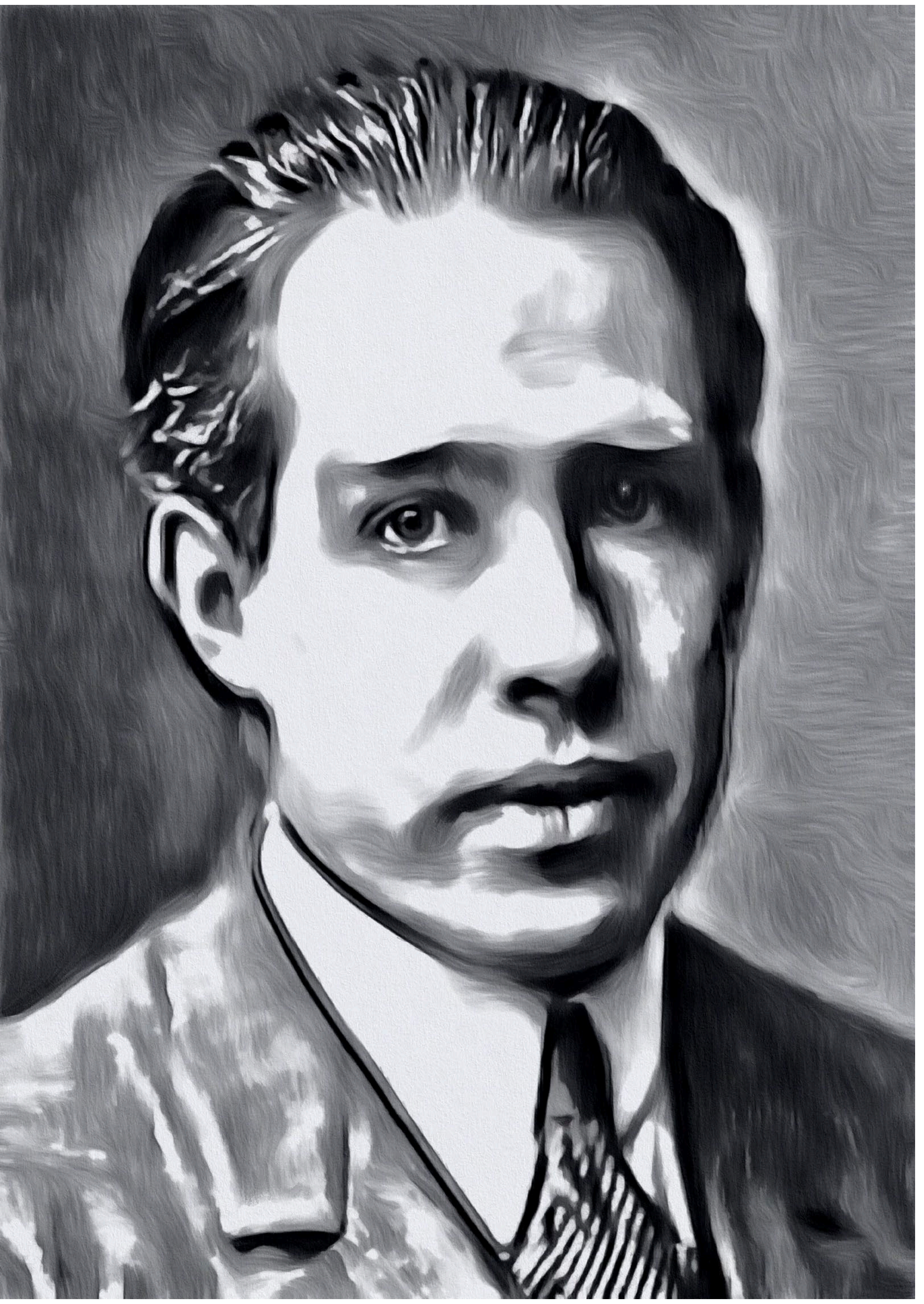
(Eingegangen am 16. November 1925.)

Die aus Heisenbergs Ansätzen in Teil I dieser Arbeit entwickelte Quantenmechanik wird auf Systeme von beliebig vielen Freiheitsgraden ausgedehnt. Die Störungstheorie wird für nicht entartete und eine große Klasse entarteter Systeme durchgeführt und ihr Zusammenhang mit der Eigenwerttheorie Hermitescher Formen nachgewiesen. Die gewonnenen Resultate werden zur Ableitung der Sätze über Impuls und Drehimpuls und zur Ableitung von Auswahlregeln und Intensitätsformeln benutzt. Schließlich werden die Ansätze der Theorie auf die Statistik der Eigenschwingungen eines Hohlraumes angewendet.

In this talk, I will not give you a historical account of how this was done

Instead, I will show you the art and the beauty of how matrix mechanics works

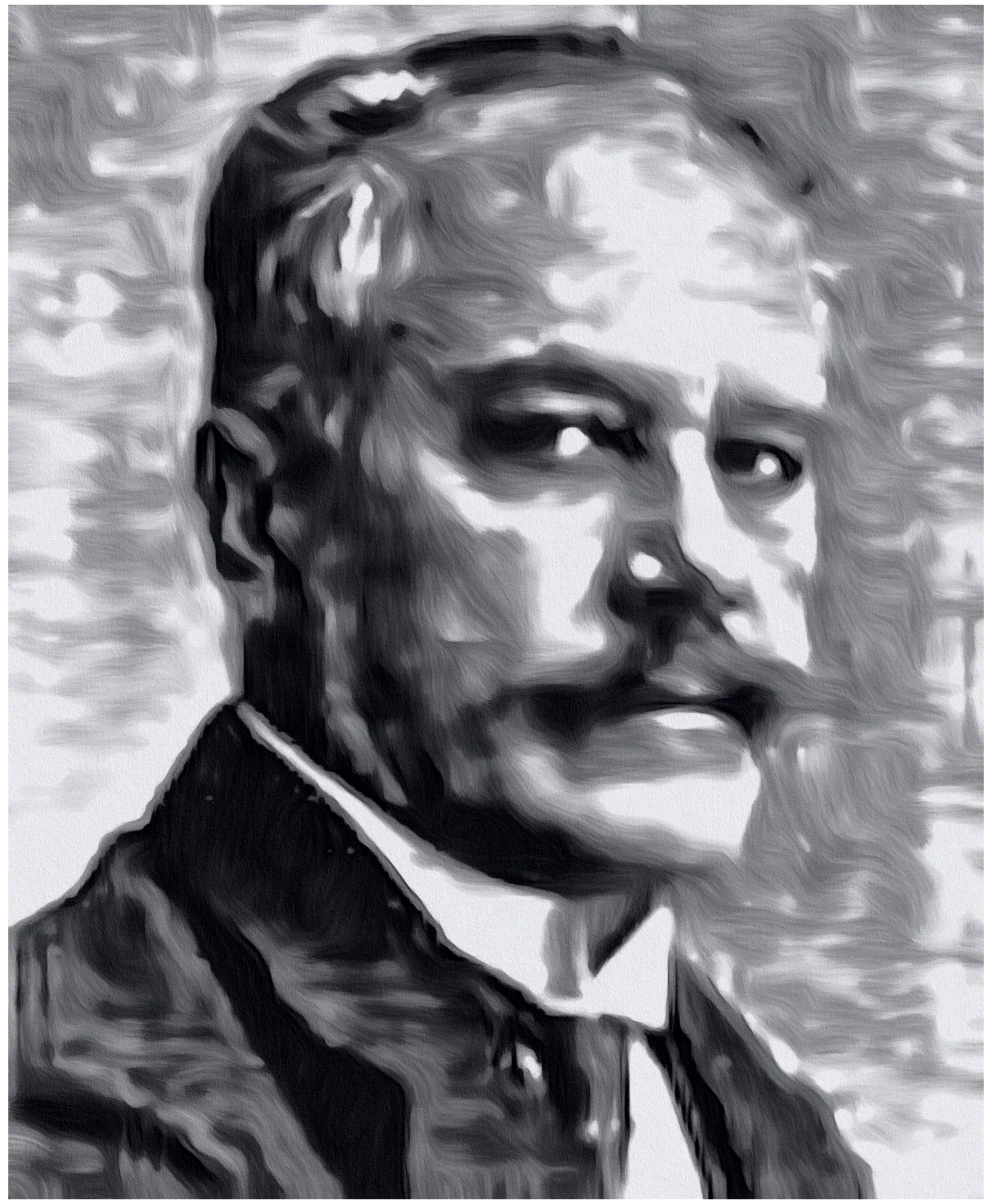
Old quantum theory in 1925



For periodic motion, one integrated the action around one period and set it equal to an integer multiplied by $\hbar$.

This produced the correct relativistic energy levels of hydrogen—a remarkable achievement!

But it failed for other atoms and become tedious to apply in many situations



Old quantum theory in 1925

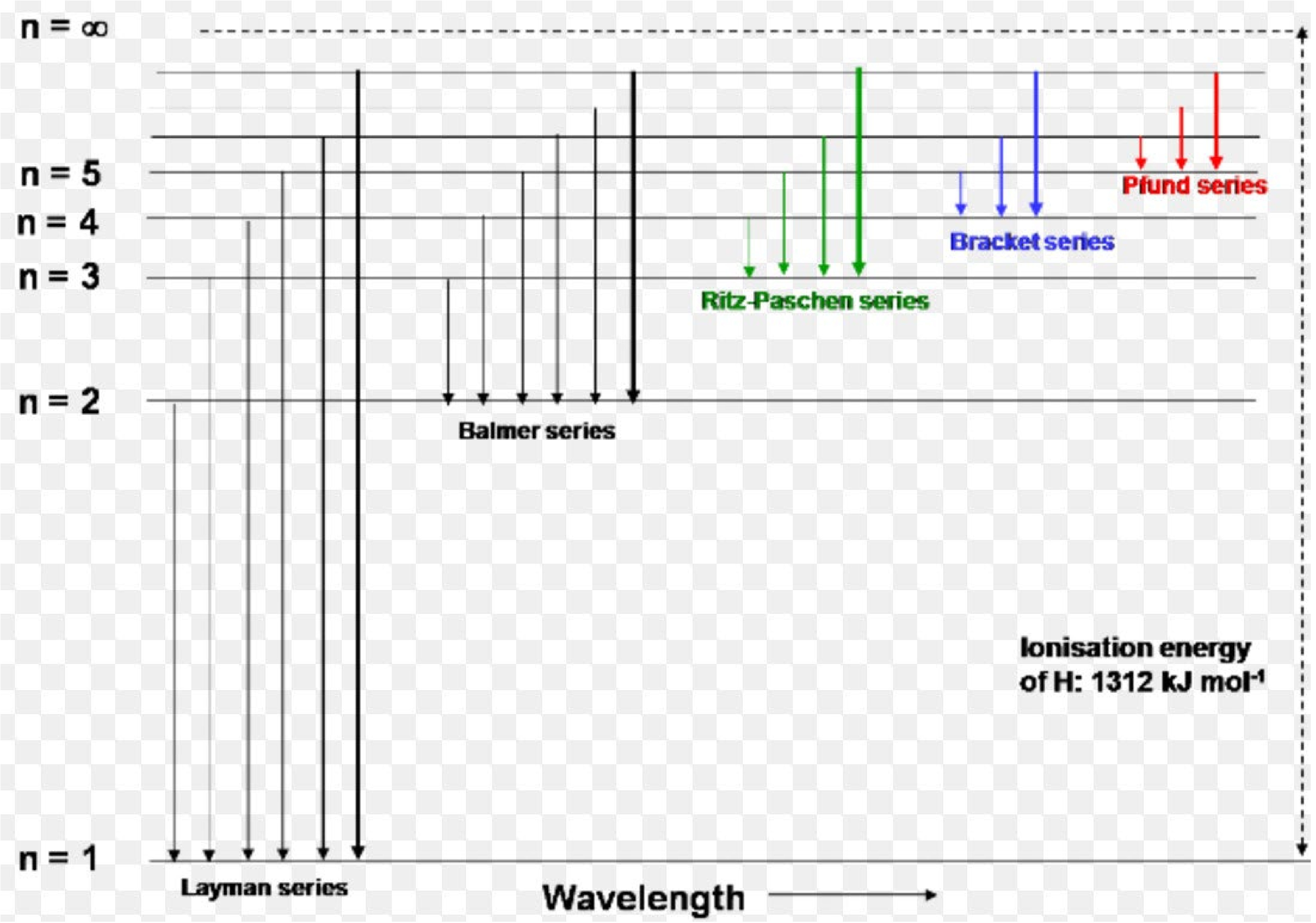
The ideas were based on Ehrenfest's notion of adiabatic invariants. These are quantities that are unchanged when the parameter in a system is changed very slowly. An example is E/ω for a harmonic oscillator if the frequency is slowly changed in time.

Old quantum theory gets the leading values for quantization correct, but does not always capture the quantum corrections

The puzzle of harmonics

In classical mechanics, we expand nonlinear periodic motion in terms of the harmonics of the fundamental.

But atomic spectra depend on the energy differences of the atomic states (Rydberg-Ritz combination principle). So, how can we expand in energy differences?



Heisenberg's solution: use matrices

Heisenberg proposed to use matrices for position $\boldsymbol{q}_{mn}$ and momentum $\boldsymbol{p}_{mn}$, whose time dependence varied harmonically in the energy differences of the two states with energies E_m and E_n.

So, we have

$$\boldsymbol{q}_{mn} = q_{mn}e^{i\omega_{mn}t} \text{ and } \boldsymbol{p}_{mn} = p_{mn}e^{i\omega_{mn}t}$$

with $\omega_{mn} = \frac{E_m - E_n}{\hbar}$. With this we find $[\boldsymbol{q}, \boldsymbol{p}] \neq 0$.

The Heisenberg equation of motion

We immediately obtain the Heisenberg equation of motion

$$\dot{\boldsymbol{q}}_{mn} = q_{mn}\frac{d}{dt}e^{i\omega_{mn}t} = i\omega_{mn}\boldsymbol{q}_{mn} = \frac{i}{\hbar}(E_m - E_n)\boldsymbol{q}_{mn} = \frac{i}{\hbar}[\boldsymbol{H},\boldsymbol{q}]_{mn}$$

because $\boldsymbol{H}$ is diagonal in this basis.

The canonical commutation relation is a constant of the motion

We use the classical equations of motion for these quantum matrices. So

$$\dot{\boldsymbol{q}} = \frac{1}{M}\boldsymbol{p} \text{ and } \dot{\boldsymbol{p}} = -\frac{dV(\boldsymbol{q})}{d\boldsymbol{q}}.$$

We use this to show that the canonical commutation relation is a constant of the motion:

$$\frac{d}{dt}[\boldsymbol{q},\boldsymbol{p}] = [\dot{\boldsymbol{q}},\boldsymbol{p}] + [\boldsymbol{q},\dot{\boldsymbol{p}}] = \frac{1}{M}[\boldsymbol{p},\boldsymbol{p}] + \left[\boldsymbol{q}, -\frac{dV(\boldsymbol{q})}{d\boldsymbol{q}}\right] = 0$$

The canonical commutation relation is a diagonal matrix

$$\frac{d}{dt}[\boldsymbol{q},\boldsymbol{p}]_{mn} = \frac{i}{\hbar}\big[\boldsymbol{H},[\boldsymbol{q},\boldsymbol{p}]\big]_{mn} = \frac{i}{\hbar}(E_m - E_n)[\boldsymbol{q},\boldsymbol{p}]_{mn} = 0$$

This means for a nondegenerate problem, when $m \neq n$ we have $E_m - E_n \neq 0$, which implies we must have $[\boldsymbol{q},\boldsymbol{p}]_{mn} = 0$. Hence, the canonical commutation relation is a diagonal matrix.

We write $[\boldsymbol{q},\boldsymbol{p}]_{mn} = c_m\delta_{mn}$.

Final derivation of the canonical commutation relation

$$\boldsymbol{p} = M\dot{\boldsymbol{q}} = \frac{i}{\hbar}M[\boldsymbol{H},\boldsymbol{q}] = \frac{iM}{\hbar}\left[\frac{\boldsymbol{p}^2}{2M} + V(\boldsymbol{q}),\boldsymbol{q}\right] = -\frac{i}{2\hbar}(\boldsymbol{p}[\boldsymbol{q},\boldsymbol{p}] + [\boldsymbol{q},\boldsymbol{p}]\boldsymbol{p})$$

Using the fact that the commutator is a diagonal matrix gives us

$$i\hbar p_{mn} = \frac{1}{2}(c_m + c_n)p_{mn}$$

Next, we assume the canonical commutation relation does not depend on the Hamiltonian. This means the form of the canonical commutation relation is the same in the eigenbasis of every Hamiltonian. The only solution that solves this requirement is $c_m = i\hbar$, so that the canonical commutation relation is proportional to the identity matrix (recall the identity matrix is the same in every basis).

Rewriting the canonical commutation relation

$$[\boldsymbol{q}, \boldsymbol{p}] = i\hbar \boldsymbol{I}$$

But $\boldsymbol{p} = M\dot{\boldsymbol{q}} = iM\omega_{mn}\boldsymbol{q}$, so we have

$$[\boldsymbol{q}, \boldsymbol{p}]_{mn} = iM \sum_{m'} (\omega_{m'n} - \omega_{mm'}) q_{mm'} q_{m'n} = i\hbar\delta_{mn}$$

Use the fact that $\boldsymbol{q}$ is Hermitian to obtain (for $m = n$)

$$\sum_{m'} \omega_{mm'} \left|q_{mm'}\right|^2 = -\frac{\hbar}{2M}$$

Solving the harmonic oscillator

$$\boldsymbol{H} = \frac{\boldsymbol{p}^2}{2M} + \frac{1}{2}M\omega^2\boldsymbol{q}^2$$

The classical equation of motion becomes $(\omega_{mn}^2 - \omega^2)q_{mn} = 0$, so when $q_{mn} \neq 0$, then $\omega_{mn} = \pm\omega$. Consider the lowest-energy state, and label it 0. Then we only have $\omega_{01} = -\omega$ and $q_{01} \neq 0$. Using the canonical commutation relation, we find that $|q_{01}|^2 = -\frac{\hbar}{2M\omega_{01}} = \frac{\hbar}{2M\omega}$.

Now, we compute H_{00} which is the ground state energy. We find

$$H_{00} = \left(\frac{M^2\omega_{01}^2}{2M} + \frac{1}{2}M\omega^2\right)|q_{01}|^2 = M\omega^2|q_{01}|^2 = \frac{1}{2}\hbar\omega$$

which is the ground-state energy. Since ω_{mn} steps up by ω the general energy is $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$. This now has the proper quantum correction.

In matrix mechanics, we calculate the spectra without determining the eigenstates, or the wavefunctions.

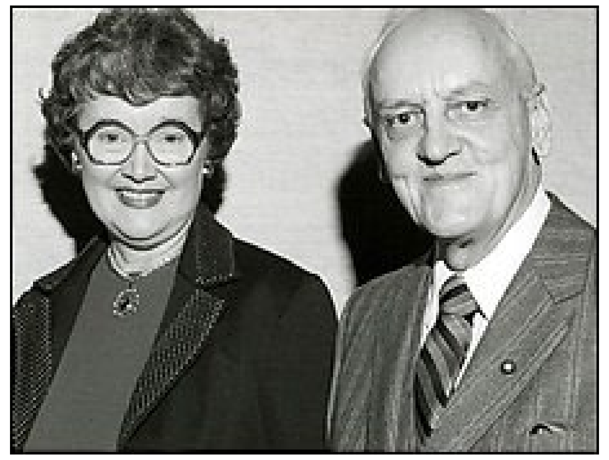
It is truly beautiful how it all fits together!

It is a pity that it only worked for the harmonic oscillator and the orbital angular momentum problems.

Thanks to

Leanne Doughty

Jason Tran



Resources

https://quantum.georgetown.domains

⟨q | Ô | m⟩

Quantum operator mechanics