

Comparison of Old Quantum Theory with Quantum Mechanics

Noel Vincze

October 2025

1 Introduction on Action-Angle variables

We start by refreshing our knowledge on action angle variables and how are they connected to motion. The main idea in action-angle variables is that we primarily consider motion only which energy is conserved. That is $H(q_i, p_i) = E$, the Hamiltonian is conserved. Hence the action (Hamilton's characteristic function) can be written as:

$$dS(q_i, t) = dW(q_i, I_i) - E dt \quad (1)$$

where I_i is a separation constant and $W(q_i, I_i)$ is Hamilton's characteristic function. The canonical transformations give rise to the following equations:

$$p_i = \frac{\partial W}{\partial q_i} \quad (2)$$

$$\phi_i = \frac{\partial W}{\partial I_i} \quad (3)$$

where ϕ_i is angle variable and conjugate to I_i , which is the action (as a variable and not as a function). In these new variables the Hamiltonian is only dependent on the action variables hence Hamilton's equation will read:

$$\dot{\phi}_i = \frac{\partial H(I_k)}{\partial I_i} \quad (4)$$

$$\dot{I}_i = -\frac{\partial H(I_k)}{\partial \phi_i} \quad (5)$$

which becomes nothing more than

$$\dot{\phi}_i = \omega_i(I_k) \quad (6)$$

$$\dot{I}_i = 0 \quad (7)$$

where ω_i is the angular frequency of the motion. From the second equation we see that I_i is a constant of motion. If we do a simple integration with respect to time on the first equation we get $\phi_i(t) = \omega_i(I_i)t + \phi_{0i}$. If we express the second equation in Poisson brackets we get an important property of the action variables. Namely we have:

$$\dot{I}_i = \{I_i, H(I_j)\} = \{I_i, I_j\} \frac{\partial H(I_k)}{\partial I_j} \quad (8)$$

Simplifying and using the equations of motions we get:

$$\{I_i, I_j\} = 0 \quad (9)$$

The action variables are involution with eachother. We define the action variables as follows:

$$I_i = \frac{1}{2\pi} \oint p_i dq_i \quad (10)$$

there is no summation on repeated indices. In this definition we see that the momentum p_i becomes coordinate dependent. To see this dependence we can rearrange the conservation of energy to get p_i . Hence we have, non magnetic and non-relativistic motion

$$p_i = n_i \sqrt{2m(E - V(q_j))} \quad (11)$$

For magnetic and relativistic motion we get the following expressions for p_i . They are

$$p_i = eA_i(q_j) + n_i \sqrt{2m(E - V(q_j))} \quad (12)$$

$$p_i = \frac{n_i}{c^2} \sqrt{(E - V(q_j))^2 - m^2 c^4} \quad (13)$$

$$p_i = eA_i(q_j) + \frac{n_i}{c^2} \sqrt{(E - V(q_j))^2 - m^2 c^4} \quad (14)$$

where n_i is the unit vector. Plugging one of these momenta (which is appropriate of the problem) into the action variable we get the following contour integral

$$I_i = \frac{1}{2\pi} \oint \sqrt{2m(E - V(q_j))} dq_i \quad (15)$$

Evaluating this integral will give us the energy of the motion in terms of the action variables. When we plug in the magnetic potential $eA_i(q_j)$ we get the magnetic flux Φ_B (One can use Stokes' theorem to prove it).

2 The Old Quantum Theory

The name old quantum theory is a bit of a misnomer because it was never a complete theory. It wasn't self-consistent either, and it was the application of

action angle variables to cyclic motion and restricting it with heuristic quantum conditions.

The main ideas that guided us to reformulate physics and discover the quantum world were the following:

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 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 now that we call photons, and then for solids, where he quantized the vibrations of ions.
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. The 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 Sommerfeld himself.
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.

To see how old quantum theory worked, first, we will consider two examples. Namely, the harmonic oscillator then the hydrogen atom and its relativistic calculations. The Sommerfeld-Wilson quantisation rule states the following:

$$\frac{1}{2\pi} \oint p_i dq_i = n_i \hbar \tag{16}$$

there is no summation on repeated indices. Applying this to the simple harmonic oscillator, we have:

$$I = \hbar = \frac{1}{2\pi} \oint \sqrt{2mE - m^2\omega^2q^2} dq \quad (17)$$

The evaluation of this integral is rather straightforward, and we get the following:

$$I = \frac{E}{\omega} \quad (18)$$

After re-ordering and using the quantum condition ($I = \hbar$), we arrive at the relation assumed by Planck and used extensively by Einstein:

$$E = \hbar\omega \quad (19)$$

If we work with n simple harmonic oscillators, we get

$$E_n = n\hbar\omega \quad (20)$$

where I indexed the energy with n , signifying that we have n oscillators. However, if we recall the correct result from quantum mechanics, we see that the zero-point energy is missing. This is an example of why the old quantum theory was set aside for quantum mechanics.

Now we turn our attention to the hydrogen problem. We are going to follow Sommerfeld's approach on this matter. The Sommerfeld-Wilson relations now read

$$\frac{1}{2\pi} \oint p_r dr = n_r \hbar \quad (21)$$

$$\frac{1}{2\pi} \oint p_\theta d\theta = n_\theta \hbar \quad (22)$$

Where p_θ was first introduced by Bohr. This integral is quite straightforward because the Hamiltonian does not have azimuthal angle dependence. Hence we have

$$\frac{1}{2\pi} \oint p_\theta d\theta = \frac{p_\theta}{2\pi} \int_0^{2\pi} d\theta = p_\theta = n_\theta \hbar \quad (23)$$

giving us Bohr's relation. The simplicity of the θ integral comes from the fact that the interaction potential has no θ dependence in the interaction of single charges/monopoles. However, when we consider higher-order multipoles such as dipoles and quadrupoles, the θ integral won't be trivial any longer. This was the case, for instance, in the Stern-Gerlach experiment ($H_{int} = -\mu B \cos(\theta)$). Now the radial part is more difficult. The Hamiltonian reads:

$$H(r, p_r, p_\theta) = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r} \quad (24)$$

Expressing p_r and plugging into the Sommerfeld-Wilson quantisation rule, we have

$$p_r = \sqrt{2mE - \frac{p_\theta^2}{r^2} + \frac{me^2}{2\pi\epsilon_0 r}} \quad (25)$$

$$n_r \hbar = \frac{1}{2\pi} \int_{r_-}^{r_+} \sqrt{2mE - \frac{p_\theta^2}{r^2} + \frac{me^2}{2\pi\epsilon_0 r}} dr \quad (26)$$

To evaluate this monstrosity, the most elegant way is to use Cauchy's residue calculus. When we do, we get the following expression

$$n_r \hbar = \frac{1}{2\pi} \left(2\pi \frac{mZe^2}{4\pi\epsilon_0 \sqrt{-2mE}} - 2\pi p_\theta \right) \quad (27)$$

Rearranging, we get for the energy

$$E_{n_r, n_\theta} = -\frac{m}{2} \left(\frac{e^2 Z}{4\pi\epsilon_0 \hbar} \right)^2 \frac{1}{(n_r + n_\theta)^2} = -\frac{E_0}{(n_r + n_\theta)^2} \quad (28)$$

Sommerfeld's result will match Bohr's when we define $n = n_r + n_\theta$. However, the big result of Sommerfeld's work is that it allows and explains the degeneracy of electron levels. This means that the fine structure splitting appears in the hydrogen spectrum. Inspired by Einstein's work on the trajectory of mercury is due to relativistic corrections, Sommerfeld used relativistic mechanics to further improve on his theory of the atom. Also with this formulation, he introduced elliptical orbits for the electron, further generalising Bohr's circular orbits. The relativistic Hamiltonian of the Hydrogen atom will read

$$H(r, p_r, p_\theta) = \sqrt{\left(p_r^2 + \frac{p_\theta^2}{r^2} \right) c^2 + m^2 c^4} - \frac{e^2}{4\pi\epsilon_0 r} \quad (29)$$

Expressing p_r we have

$$p_r = \sqrt{\frac{E^2}{c^2} - m^2 c^2 + \frac{EZe^2}{2\pi\epsilon_0 c^2 r} + \frac{Z^2 e^4}{16\pi^2 \epsilon_0^2 c^2 r^2} - \frac{p_\theta^2}{r^2}} \quad (30)$$

Plugging this into the Sommerfeld-Wilson formula and using residue calculus to evaluate it we get:

$$n_r \hbar = \frac{1}{2\pi} \int_{r_-}^{r_+} \sqrt{\frac{E^2}{c^2} - m^2 c^2 + \frac{EZe^2}{2\pi\epsilon_0 c^2 r} + \frac{Z^2 e^4}{16\pi^2 \epsilon_0^2 c^2 r^2} - \frac{p_\theta^2}{r^2}} dr \quad (31)$$

$$n_r \hbar = \frac{1}{2\pi} \left(2\pi \frac{EZe^2}{4\pi\epsilon_0 \sqrt{m^2 c^4 - E^2}} - 2\pi \sqrt{p_\theta^2 - \left(\frac{Ze^2}{4\pi\epsilon_0 c} \right)^2} \right) \quad (32)$$

Then, using this relation with Bohr's azimuthal quantisation we find the energy to be

$$E_{n_r, n_\theta} = mc^2 \left[1 + \left(\frac{\alpha Z}{n_r + \sqrt{n_\theta^2 - \alpha^2 Z^2}} \right)^2 \right]^{-1/2} \quad (33)$$

where I introduced α for the fine structure constant, which is defined as

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \quad (34)$$

When we do a Taylor expansion of Sommerfeld's relativistic hydrogen atom in α we get back the low energy equation of the hydrogen atom. Namely we find Bohr's result again in the form of

$$E_{n_r, n_\theta} \approx mc^2 - \frac{mc^2 Z^2 \alpha^2}{2(n_r + n_\theta)^2} + \frac{mc^2 Z^4 \alpha^4}{2(n_r + n_\theta)^4} \left(\frac{3}{4} - \frac{n_r + n_\theta}{n_\theta} \right) \quad (35)$$

The truly remarkable part of this work is that firstly relativistic considerations actually split the spectral lines because now there is an energy gap between degenerate electron states, namely $\Delta E = mc^2 Z^4 \alpha^4 / 32$ and whilst this new model he predicted the fine structure splitting of Helium spectra (experimentally confirmed by F. Paschen), secondly, he got to these results in 1916 a full 20 years sooner to the discovery of the correct quantum mechanical formula derived by P. Dirac in 1936.

As remarkable and cutting-edge as the Bohr-Sommerfeld model of the Hydrogen it had many limitations. Namely

1. It describes only one relativistic electron in elliptical orbit
2. Does not explain neither the Zeeman nor the Stark effect
3. Only applicable to circular motion (this feature is built in since we work with Action-Angle variables, which only describe periodic motion)

Furthermore, in 1922, when the Stern-Gerlach experiment was carried out, O. Stern formulated this experiment because he took the polar quantization literally, that is,

$$\frac{1}{2\pi} \oint p_\phi d\phi = n_\phi \hbar \quad (36)$$

With this quantization rule included, now we have quantized all three degrees of freedom of a particle in a spherical potential. This experiment ruled in favor of quantum mechanics and demonstrated that the spatial quantization was real. Even though the correct interpretation arrived a year later in the form of spin precession.

3 The fall of Old Quantum Theory

In this section, we are going to analyse the final results of the old quantum theory with the results of quantum mechanics and discuss the differences of interpretation and how they arise in the equations for energy.

First of all, the simple harmonic oscillator. From the old and new theories we have

$$E_{old}(n) = n\hbar\omega \quad (37)$$

$$E_{new}(n) = \hbar\omega \left(n + \frac{1}{2} \right) \quad (38)$$

As we can see from quantum mechanics, we have an extra term, namely the zero-point energy term, that arises from the non-commutativity of position and momentum operators ($[x, -i\hbar\nabla] = i\hbar$). Furthermore, it also says that even when particles are in their ground state, they have a little energy with which they can wiggle and jiggle away. This means that quantum particles will know no true rest.

Secondly, and most importantly, the energy of the Hydrogen atom. We have

$$E_{old}(n_r, n_\theta) = mc^2 \left[1 + \left(\frac{\alpha Z}{n_r + \sqrt{n_\theta^2 - \alpha^2 Z^2}} \right)^2 \right]^{-1/2} \quad (39)$$

$$E_{new}(n_r, j) = mc^2 \left[1 + \left(\frac{\alpha Z}{n_r + \sqrt{(j + \frac{1}{2})^2 - \alpha^2 Z^2}} \right)^2 \right]^{-1/2} \quad (40)$$

The new expression of Dirac's now includes the spin of fermions, which is not possible through the Sommerfeld-Wilson quantisation rule. Furthermore, another big distinction of the quantum numbers, while in the old quantum theory the set of (n_r, n_θ, n_ϕ) are independent of each other hence $n_i \in \mathbb{R}^+$, in Dirac's theory the set of quantum numbers (n_r, j, m_j) are related to each other in the following way: $n_r \in \mathbb{R}^+$, $j \in \{0, 1, \dots, n_r - 1\}$, while $m_j \in \{-j, -j+1, \dots, j-1, j\}$. With this, Dirac completed the theory of the atom that had been in the making for well over 20 years. Furthermore, Dirac also predicted the negative energy states of particles, now called anti-particles.

As a final note, W. Heisenberg's work on the development of matrix mechanics was heavily influenced by Action-Angle variables. This formulation of classical mechanics has been at the core of physics in the early 20th century, both quantum and classical. Heisenberg's genius was to combine 3 powerful mathematical techniques to describe quantum mechanics. These were Action-Angle variables, Fourier series and using discrete operators instead of the continuous ones. Heisenberg's work was cast into its final form by M. Born and P. Jordan in the same year.

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-wQj11vVxch-RPQUIUOHX88eeNGzVH&pp=0gcJCa4E0CosWNin