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Sommerfeld's elliptical atomic orbits revisited—A useful preliminary to the study of quantum mechanics

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The Bohr-Sommerfeld atomic model is recast in the language of wave-particle duality and it is shown that requirements equivalent to the Sommerfeld-Wilson quantisation conditions arise naturally in this context. It is suggested that treating the one-electron atom in this way provides a useful introduction for students prior to encountering the more formal analysis based on the solution of the Schrödinger equation. © 2014 American Association of Physics Teachers.
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I. INTRODUCTION

Sommerfeld's extension of the Bohr Model¹ to elliptical orbits in 1915, later described in detail in his book *Atomic Structure and Spectral Lines* (1919),² predated de Broglie's hypothesis of wave-particle duality (1924) by almost a decade. The development of quantum mechanics during 1925 and 1926 followed rapidly on the heels of de Broglie's thesis and his subsequent papers so that little attention was brought to bear on the significance of wave-particle duality for the "old quantum theory."

Furthermore, Sommerfeld and others involved in the development of the old quantum theory in those years were all experts in the Hamiltonian formulation of classical dynamics. It was natural, therefore, that they would express the generalisation of the quantum conditions in that language, specifically in terms of relations between "canonically conjugate" variables, which is usually the way this material is presented in textbooks since that time. Specifically the original quantization rules, proposed independently by Wilson,³ Ishiwara,⁴ and Sommerfeld,⁵ take the form

$$\oint p_k dq_k = n_k h, \quad (1)$$

where p_k is the "generalized momentum" corresponding to the "generalized canonical coordinate" q_k , n_k is an integer, and h is the Planck constant. In the context of elliptical orbits, the q_k 's are the radial and angular coordinates r and θ , while the corresponding generalized momenta are momentum and angular momentum, respectively.

Physics students today, however, are unlikely to have encountered Hamiltonian mechanics prior to their first exposure to quantum ideas. On the other hand, these same students would have to be *au fait* with wave-particle duality before proceeding to a formal study of quantum mechanics. What follows below is an attempt to recast Sommerfeld's atomic model in a language more suitable to students today. It is suggested that the presentation of this treatment as a starting point for the study of the quantum mechanics of one-electron atomic systems would be beneficial for learners. In particular, it should help to clarify which aspects of quantum theory arise naturally from wave-particle duality and which are intrinsic to the particularities of the formal theory.

II. DE BROGLIE'S REINTERPRETATION OF THE BOHR MODEL

In his celebrated 1924 doctoral dissertation,⁶ de Broglie pointed out,

"...that a trajectory of a moving particle is identical to a ray of a phase wave, along which frequency is constant (because total energy is constant) and with variable velocity, whose value we shall not attempt to calculate. Propagation is, therefore, analogous to a liquid wave in a channel closed on itself but of variable depth. It is physically obvious, that to have a stable regime, the length of the channel must be resonant with the wave; in other words, the points of a wave located at whole multiples of the wave length λ , must be in phase. The resonance condition is $l = n\lambda$ if the wave length is constant... Thus, the resonance condition can be identified with the stability condition from quantum theory. This beautiful result... constitutes the best justification that we can give for our attack on the problem of interpreting quanta."

He then went on to apply wave-particle duality to the particular case of electrons (mass m_e) undergoing circular Bohr orbits (radius R and angular frequency ω) in an atom and showed that the electron's angular momentum was given by

$$pR = m_e \omega R^2 = n \frac{h}{2\pi}, \quad (2)$$

where n is a non-zero integer.

In order to give a context for what follows in this paper, we first restate de Broglie's idea above in somewhat different terms. Consider a harmonic wave (wavelength λ and period T) moving on a circular path of radius R . We can write the disturbance of this wave at an arbitrary point on the circle (Fig. 1) as

$$\Psi(s, t) = Ae^{i(ks - \omega t)} \quad (3)$$

or

$$\Psi(\phi, t) = Ae^{i(kR\phi - \omega t)}, \quad (4)$$

where $k = 2\pi/\lambda$, $\omega = 2\pi/T$, and the wavespeed is $v = \omega/k$. Note that, since the function Ψ is intended in due course to represent a de Broglie wave-particle, the "disturbance" is entirely abstract.

For this wave to have what de Broglie called "a stable regime"—for a coherent wave pattern to be set up—the wave must return exactly in phase after completing one revolution. In other words, $\Psi(\phi + 2\pi, t) = \Psi(\phi, t)$ or $Ae^{i(kR\phi + 2\pi kR - \omega t)} = Ae^{i(kR\phi - \omega t)}$. Thus, the requirement for a stable (circular) wave pattern is $kR = 2\pi R/\lambda = n$, with n a non-zero integer. Invoking the de Broglie hypothesis for the momentum of a particle $p = h/\lambda$, this yields $2\pi pR/h = n$ or

$$pR = n \frac{h}{2\pi} \equiv n\hbar, \quad (5)$$

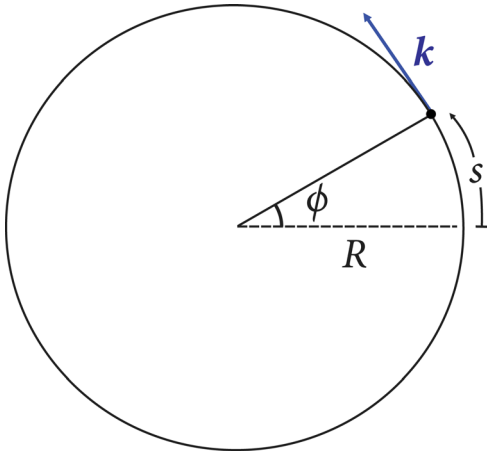


Fig. 1. Wave on a circular path.

which is equivalent to the expression for the angular momentum of the particle orbiting on a circular path quoted from de Broglie above [Eq. (2)]. Thus, the quantum condition applied by Bohr to the hydrogen atom is seen by de Broglie as being equivalent to the requirement that the electron wave generates a stable wave pattern on the circle.

Applied to a particle in circular orbit under any inverse-square-law force (with potential energy given by $U(r) = -\kappa/r$, where κ is constant), this result yields the Bohr quantization of energy E , angular momentum L , and orbit radius r ; namely,

$$E_n = -\frac{m_r \kappa^2}{2\hbar^2} \frac{1}{n^2}, \quad (6)$$

$$L_n = n\hbar, \quad (7)$$

and

$$r_n = \frac{\hbar^2}{m_r \kappa} n^2. \quad (8)$$

Here, $\kappa = Ze^2/4\pi\epsilon_0$ in the case of a one-electron atom and m_r is the reduced mass of the system.

III. CLASSICAL ELLIPTICAL ORBITS

Sommerfeld and his contemporaries were troubled by the fact that the Bohr quantum atom appeared to demand circular orbits only, and in particular by the consequence that for any fixed energy there is only one possible value of the corresponding angular momentum (or two of equal magnitude if one allows for clockwise and counter-clockwise rotations). From the classical Kepler problem, it follows that for a fixed energy in an elliptical orbit (Fig. 2) there are an infinite number of possible angular momentum values, each depending on the eccentricity of the elliptical path involved. The total energy of a particle in an elliptical orbit depends only on the semi-major axis a and is given by

$$E = -\frac{\kappa}{2a}, \quad (9)$$

while the angular momentum depends on the semi-minor axis b according to

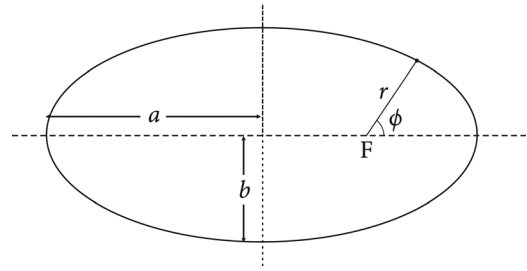


Fig. 2. Particle on an elliptical path under a force centered at the focus.

$$L^2 = -2m_r E b^2. \quad (10)$$

Furthermore, evidence based on observation of atomic spectra available at the time suggested a more complicated picture than Bohr's, which Sommerfeld's model was designed to explain.

The problem of treating a particle in an elliptical orbit as a de Broglie wave is somewhat more complicated than in the case of circular motion. For one thing, the wave amplitude depends on two spatial variables so that $\Psi = \Psi(r, \phi, t)$, with the two (polar) spatial variables (r, ϕ) related by the equation of the ellipse:

$$r = \frac{b^2}{a(1 + e \cos \phi)} = \frac{a(1 - e^2)}{1 + e \cos \phi}, \quad (11)$$

where $e = \sqrt{1 - b^2/a^2}$ is the eccentricity of the ellipse. In addition, the magnitude of the particle's momentum, potential energy, and kinetic energy are all continuously changing throughout the orbit. Conservation of energy, using Eq. (9) above, gives

$$\frac{p^2}{2m_r} + U(r) = \frac{p^2}{2m_r} - \frac{\kappa}{r} = -\frac{\kappa}{2a}, \quad (12)$$

from which we get

$$p^2 = m_r \kappa \left(\frac{2}{r} - \frac{1}{a} \right) = m_r \kappa \left[\frac{2a(1 + e \cos \phi)}{b^2} - \frac{1}{a} \right], \quad (13)$$

$$U = -\frac{\kappa(1 + e \cos \phi)}{a(1 - e^2)}, \quad (14)$$

and

$$T = \frac{\kappa(1 + e^2 + 2e \cos \phi)}{2a(1 - e^2)}. \quad (15)$$

Finally, using Eqs. (9) and (10), the semi-major axis can be written as

$$a = \frac{L^2}{m_r \kappa (1 - e^2)}. \quad (16)$$

IV. APPLICATION OF THE DE BROGLIE HYPOTHESIS TO ELLIPTICAL ORBITS

Because the magnitude of the momentum of the particle in an elliptical orbit varies with r and ϕ , a function in the form of Eq. (3) cannot represent the particle. Indeed, the

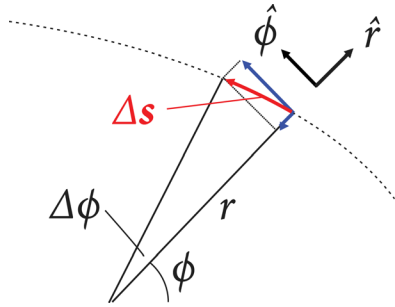


Fig. 3. Plane polar coordinates used in text.

corresponding de Broglie wave must be considered to have a wavelength that varies continuously around the orbit. However, over a small enough time interval Δt , during which $r \rightarrow r + \Delta r$ and $\phi \rightarrow \phi + \Delta\phi$, p can be considered to be sensibly constant, in which case the wave-particle can be represented by

$$\Psi(r, \phi, t) = A(r, \phi)e^{i(k_r \Delta s - \omega \Delta t)}, \quad (17)$$

where $A(r, \phi)$ is real. It is convenient to resolve the motion into the two independent orthogonal directions, indicated by the \hat{r} and $\hat{\phi}$ directions in Fig. 3, so that

$$\begin{aligned} \Psi(r, \phi, t) &= A(r, \phi)e^{i[k_r(\Delta s)_r + k_\phi(\Delta s)_\phi - \omega(\Delta t)]} \\ &= A(r, \phi)e^{i(k_r \Delta r + k_\phi r \Delta\phi - \omega \Delta t)} \end{aligned} \quad (18)$$

and the wave at the point (r, ϕ) can be represented by a product of radial and angular functions as

$$\Psi(r, \phi, t) = A_r e^{ik_r \Delta r} A_\phi e^{irk_\phi \Delta\phi} e^{-i\omega \Delta t}. \quad (19)$$

As in the case of a circular orbit, the condition for a stable wave pattern in this case is that the wave should return in phase after one full revolution of the orbit. In this case, we require

$$\oint r k_\phi d\phi = 2\pi n_\phi \quad \text{and} \quad \oint k_r dr = 2\pi n_r, \quad (20)$$

where n_ϕ and n_r are integers (not necessarily equal) and the integration is over one complete cycle. Again, we invoke the de Broglie hypothesis $p = h/\lambda$ to get $k = 2\pi/\lambda = 2\pi p/h$, and thus

$$\oint p_\phi r d\phi = n_\phi h \quad \text{and} \quad \oint p_r dr = n_r h. \quad (21)$$

These are precisely the original quantum conditions proposed by Wilson, Ishiwara, and Sommerfeld [recall Eq. (1) above], derived here using de Broglie wave concepts only.

The first of the conditions in Eq. (21) reduces to Eq. (5) in the case of circular orbits (corresponding to $n_r = 0$), the integrand being identified as the angular momentum of the particle $L = |\mathbf{r} \times \mathbf{p}| = rp_\phi$. Since L is a constant of the motion, the first condition therefore becomes

$$L \oint d\phi = L(2\pi) = n_\phi h \quad \text{or} \quad L = n_\phi \hbar. \quad (22)$$

A negative value of n_ϕ can be interpreted as corresponding to rotation in the opposite sense (clockwise rather than

counterclockwise in Fig. 2). The possibility of n_ϕ being zero was, to quote Pauling and Wilson,⁷ “somewhat arbitrarily excluded, on the basis of the argument that the corresponding orbit is a degenerate line ellipse which would cause the electron to strike the nucleus.”

To integrate the second condition in Eq. (21), one notes that

$$p_r = m_r \frac{dr}{dt} = m_r \frac{dr}{d\phi} \frac{d\phi}{dt} = \frac{1}{r^2} \left(m_r r^2 \frac{d\phi}{dt} \right) \frac{dr}{d\phi} = \frac{L}{r^2} \frac{dr}{d\phi}, \quad (23)$$

so that

$$\oint p_r dr = \oint \frac{L}{r^2} \left(\frac{dr}{d\phi} \right)^2 d\phi = n_r h. \quad (24)$$

Then, using Eq. (11) the integral can be evaluated⁸ to give

$$n_r h = e^2 L \int_0^{2\pi} \frac{\sin^2 \phi d\phi}{(1 + e \cos \phi)^2} = 2\pi L \left(\frac{1}{\sqrt{1 - e^2}} - 1 \right), \quad (25)$$

and substituting $L = n_\phi \hbar$ from Eq. (22) then leads to

$$\sqrt{1 - e^2} = \frac{n_\phi}{n_r + n_\phi} = \frac{b}{a}. \quad (26)$$

We now replace n_r and n_ϕ by two new integers $m = \pm n_\phi$ and $n = n_r + n_\phi$ so that we can write $\sqrt{1 - e^2} = b/a = |m|/n$. Thus, the only allowed orbits are those with (quantized) eccentricity given by

$$e_{nm} = \sqrt{1 - \frac{m^2}{n^2}}, \quad (27)$$

where n and m are integers satisfying $n > 0$ and $-n < m < n$ (with $m \neq 0$). Figure 4 shows the predicted orbits for $n = 4$. Note that the circular ($\epsilon = 0$) orbits have $m = \pm n$, giving $n_r = 0$, as expected. (The ground state is given by $n = 1$, $m = \pm 1$.)

Finally, using Eqs. (9), (16), and (22), we can find the (quantized) energy, angular momentum, and the semi-major and minor axes as a function of the quantum numbers n and m :

$$E_{nm} = -\frac{m_r k^2}{2\hbar^2} \frac{1}{n^2}, \quad (28)$$

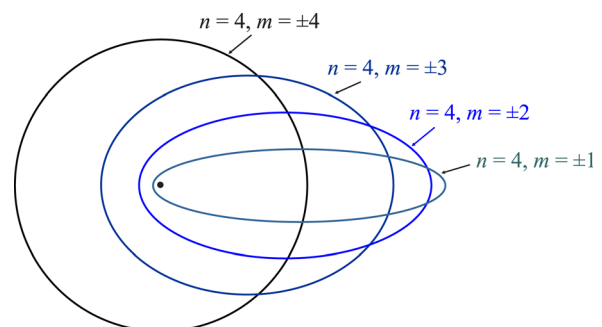


Fig. 4. Sommerfeld elliptical orbits for the case $n = 4$.

$$L_{nm} = m\hbar, \quad (29)$$

$$a_{nm} = \frac{\hbar^2}{m_r \kappa} n^2, \quad (30)$$

and

$$b_{nm} = \frac{m}{n} a_n = mn \frac{\hbar^2}{m_r \kappa}. \quad (31)$$

V. A NOTE ON A FULL QUANTUM-MECHANICAL TREATMENT

The central field is of course a spherically symmetric potential, but in classical dynamics, and by extension in the old quantum theory, initial conditions remove this symmetry and force the motion to take place in a plane. Sommerfeld did attempt to extend his model to three dimensions by postulating a third quantum condition: $\oint p_\theta d\theta = n_\theta h$. A consequence of this postulate is that when there is a preferred direction in the system (for example, by the application of an external field to the atom), this condition imposes a requirement that the planes of the elliptical orbits take on only certain orientations—the phenomenon of “space quantization.”

Sommerfeld’s analysis was quickly overtaken by the development of formal quantum mechanics by Heisenberg, Jordan, Born, Dirac, and others, and by Schrödinger’s non-relativistic treatment of the hydrogen atom in 1926.⁹ Application of the Schrödinger equation gave rise to the same energy levels as in the Bohr and Sommerfeld

approaches but the solutions were found to depend on θ as well as r and ϕ . While the Schrödinger method overcomes the limitations in the Bohr-Sommerfeld description, many of the general features associated with the quantum theory of atoms are anticipated in the earlier model. Thus, the analysis outlined in this paper can provide a useful transition for students in going from the simple Bohr model to the full solution of the Schrödinger equation when applied to a one-electron atom.

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