



ELSEVIER

Contents lists available at ScienceDirect

Studies in History and Philosophy
of Modern Physicsjournal homepage: www.elsevier.com/locate/shpsbThe trouble with orbits: The Stark effect in the old and the new
quantum theory[☆]Anthony Duncan^a, Michel Janssen^{b,*}^a Department of Physics and Astronomy, University of Pittsburgh, United States^b Program in the History of Science, Technology, and Medicine, University of Minnesota, United States

ARTICLE INFO

Article history:

Received 7 April 2014

Received in revised form

25 July 2014

Accepted 30 July 2014

Available online 26 September 2014

Keywords:

Stark effect

Bohr–Sommerfeld theory

Hamilton–Jacobi theory

Epstein

Wave mechanics

WKB approximation

ABSTRACT

The old quantum theory and Schrödinger's wave mechanics (and other forms of quantum mechanics) give the same results for the line splittings in the first-order Stark effect in hydrogen, the leading terms in the splitting of the spectral lines emitted by a hydrogen atom in an external electric field. We examine the account of the effect in the old quantum theory, which was hailed as a major success of that theory, from the point of view of wave mechanics. First, we show how the new quantum mechanics solves a fundamental problem that one runs into in the old quantum theory with the Stark effect. It turns out that, even without an external field, it depends on the coordinates in which the quantum conditions are imposed which electron orbits are allowed in a hydrogen atom. The allowed energy levels and hence the line splittings are independent of the coordinates used but the size and eccentricity of the orbits are not. In the new quantum theory, this worrisome non-uniqueness of orbits turns into the perfectly innocuous non-uniqueness of bases in Hilbert space. Second, we review how the so-called WKB (Wentzel–Kramers–Brillouin) approximation method for solving the Schrödinger equation reproduces the quantum conditions of the old quantum theory amended by some additional half-integer terms. These extra terms remove the need for some arbitrary extra restrictions on the allowed orbits that the old quantum theory required over and above the basic quantum conditions.

© 2014 Elsevier Ltd. All rights reserved.

When citing this paper, please use the full journal title *Studies in History and Philosophy of Modern Physics*

1. Introduction

In March of 1916, Epstein (1916a, 1916b) and Schwarzschild (1916) showed that the old quantum theory of Bohr (1913) and Sommerfeld (1915a, 1915b, 1916) can account for an effect discovered by and named after Stark (1913), the splitting of the Balmer lines when a hydrogen atom is placed in an external electric field.¹ This result was hailed as a tremendous success for the old quantum theory. Epstein (1916a, p. 150) boasted that “the reported results prove the correctness of Bohr's atomic model with such striking evidence that even our conservative colleagues

cannot deny its cogency.” In the conclusion of the first edition of his *Atombau und Spektrallinien*, the bible of the old quantum theory, Sommerfeld (1919, p. 458) called the theory's explanation of the Stark effect one of “the most impressive achievements in our field” and a “capstone on the edifice of atomic physics.”

However, as we noted in an earlier paper (Duncan & Janssen, 2014), the old quantum theory's explanation of the Stark effect was not without its share of problems. These problems were solved when, shortly after the arrival of Schrödinger's (1926a) wave mechanics, Schrödinger (1926b) and Epstein (1926) produced an account of the Stark effect in the new theory. In this paper, we focus on two of these problems and show how they are resolved in wave mechanics.

First, we show how the new quantum mechanics takes care of a fundamental problem in the old quantum theory that manifests itself glaringly in the Stark effect. The allowed orbits of the electron in the hydrogen atom, with or without an external field, depend on the coordinates in which the quantum conditions are imposed. The allowed energy levels and hence the line splittings do not depend on the coordinates used but the size and

[☆]We dedicate this paper to the memory of Philip M. Stehle (1919–2013).

* Corresponding author at: Tate Lab of Physics, 116 Church St. SE, Minneapolis, MN 55455, USA.

E-mail addresses: tony@dectony.phyast.pitt.edu (A. Duncan),janss011@umn.edu (M. Janssen).¹ For an account of the developments leading up to this result, see Duncan & Janssen (2014), which, in turn, draws on Kragh (2012) and especially Eckert (2013). For an English version, see Eckert (2014).

eccentricity of the elliptical orbits do. In the new quantum theory, this worrisome non-uniqueness of orbits turns into the perfectly innocuous non-uniqueness of bases in Hilbert space.

Second, we show how wave mechanics eliminates the need for extra restrictions on the allowed orbits over and above the basic quantum conditions in the old quantum theory. We review how the so-called WKB approximation method for solving the Schrödinger equation, named after [Wentzel \(1926\)](#), [Kramers \(1926\)](#) and [Brillouin \(1926\)](#), reproduces the quantum conditions of the old quantum theory amended by some additional half-integer terms. With these additional terms, there is no need anymore for extra restrictions on the allowed orbits.

We will proceed as follows. In [Section 2](#), we use the old quantum theory to find the formula for the energy levels for the first-order Stark effect in hydrogen, i.e., the energy of the allowed electron orbits in a hydrogen atom in a weak electric field, to first order in the strength of that field. We show that the old quantum theory calls for some arbitrary restrictions on the allowed orbits over and above the basic quantum conditions. In [Section 3](#), we present the problem of the non-uniqueness of orbits in the old quantum theory. In [Section 4](#), we sketch how the formula for the energy levels in the Stark effect is derived in wave mechanics. We only present the first part of this derivation in detail. This suffices to show how wave mechanics avoids the need for extra restrictions on the allowed quantum states. In [Section 5](#), we show how the problem of the non-uniqueness of orbits in the old quantum theory is solved in the new quantum mechanics. In [Section 6](#), we use the WKB method to find approximate solutions to the Schrödinger equation to recover the quantum conditions of the old quantum theory from wave mechanics with correction terms of $\frac{1}{2}$. These correction terms remove the need for extra restrictions on the allowed orbits in the old quantum theory. In [Section 7](#), we summarize our conclusions.

2. The Stark effect in the old quantum theory

In Cartesian coordinates (x, y, z) , the Hamiltonian for an electron (reduced mass μ , charge $-e$) in a hydrogen atom in an external electric field \mathcal{E} in the z -direction is given by (in Gaussian units)

$$H = \frac{p^2}{2\mu} - \frac{e^2}{r} + e\mathcal{E}z, \quad (1)$$

where $p^2 \equiv p_x^2 + p_y^2 + p_z^2$, with (p_x, p_y, p_z) the momenta conjugate to the coordinates (x, y, z) .

We switch to parabolic coordinates (ξ, η, φ) , related to (x, y, z) via ([Kramers, 1919, p. 301, Eq. \(43\)](#))²

$$z = \frac{\xi - \eta}{2}, \quad x + iy = \sqrt{\xi\eta}e^{i\varphi}. \quad (2)$$

This coordinate transformation is illustrated in [Fig. 1](#). It follows from [Eq. \(2\)](#) that

$$r^2 = x^2 + y^2 + z^2 = \xi\eta + \frac{(\xi^2 - 2\xi\eta + \eta^2)}{4} = \frac{(\xi + \eta)^2}{4}, \quad (3)$$

or

$$r = \frac{\xi + \eta}{2}. \quad (4)$$

² [Epstein \(1916b, p. 495, Eqs. \(19\) & \(20\)\)](#) defined parabolic coordinates slightly differently. In the notation of [Eq. \(2\)](#), he set $z = (\xi^2 - \eta^2)/2$ and $\sqrt{x^2 + y^2} = \xi\eta$. Moreover, Epstein called x what we call z and y what we call $\sqrt{x^2 + y^2}$. The quantity $r \equiv \sqrt{x^2 + y^2}$ in Epstein's notation (i.e., with $x = (\xi^2 - \eta^2)/2$ and $y = \xi\eta$) is thus equal to $r \equiv \sqrt{x^2 + y^2 + z^2}$ in our notation. Instead of [Eq. \(4\)](#) below, Epstein found $r = (\xi^2 + \eta^2)/2$.

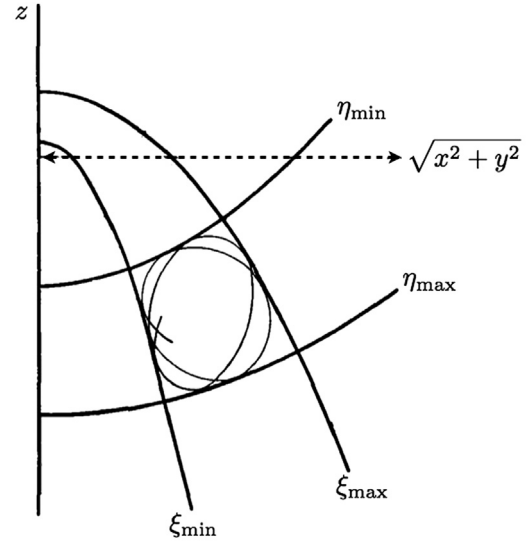


Fig. 1. Parabolic coordinates. This figure is taken from [Epstein \(1916b, p. 498\)](#) but the labeling has been changed to reflect the definition of the coordinate transformation $(x, y, z) \rightarrow (\xi, \eta, \varphi)$ as given in [Eq. \(2\)](#), which follows [Kramers \(1919, p. 301, Eq. \(43\)\)](#) rather than [Epstein \(1916b, p. 495, Eqs. \(19\) & \(20\)\)](#). The figure shows what Epstein calls a “meridian plane” ([Epstein, 1916b, p. 495, Eqs. \(19\) & \(20\)](#)), a plane through the z -axis and the position of the electron. This plane rotates around the z -axis as the electron orbits the nucleus. Within this plane, the electron stays between ξ_{\min} and ξ_{\max} and between η_{\min} and η_{\max} .

In parabolic coordinates the Hamiltonian in [Eq. \(1\)](#) is given by

$$H = \frac{1}{2\mu} \left(\frac{4}{\xi + \eta} (p_\xi \xi p_\xi) + \frac{4}{\xi + \eta} (p_\eta \eta p_\eta) + \frac{1}{\xi \eta} p_\varphi^2 \right) - \frac{2e^2}{\xi + \eta} + \frac{1}{2} e\mathcal{E}(\xi - \eta), \quad (5)$$

where $(p_\xi, p_\eta, p_\varphi)$ are the momenta conjugate to (ξ, η, φ) . In the old quantum theory, as in classical mechanics, $p_\xi \xi p_\xi = \xi p_\xi^2$ and $p_\eta \eta p_\eta = \eta p_\eta^2$. The reason we wrote these products the way we did in [Eq. \(5\)](#) is that in wave mechanics p_ξ becomes a differential operator, differential operator, $(\hbar/i)\partial/\partial\xi$ (with $\hbar \equiv h/2\pi$, where h is Planck's constant) that does not commute with multiplication by ξ .

Using E to denote energy, we write

$$H = E = \alpha_1, \quad (6)$$

where α_1 is some negative constant. Substituting α_1 for H in [Eq. \(5\)](#), multiplying both sides of by $2\mu(\xi + \eta)$, and making the substitutions

$$p_\xi \rightarrow \frac{\partial S}{\partial \xi}, \quad p_\eta \rightarrow \frac{\partial S}{\partial \eta}, \quad p_\varphi \rightarrow \frac{\partial S}{\partial \varphi}, \quad (7)$$

related to a canonical transformation generated by an as yet unknown function S , known as *Hamilton's principal function* ([Goldstein, Poole, & Safko, 2002, p. 431](#)), we obtain the Hamilton–Jacobi equation for this system in parabolic coordinates in the following form:³

$$4\xi \left(\frac{\partial S}{\partial \xi} \right)^2 + 4\eta \left(\frac{\partial S}{\partial \eta} \right)^2 + \left(\frac{1}{\xi} + \frac{1}{\eta} \right) \left(\frac{\partial S}{\partial \varphi} \right)^2 - 4\mu e^2 + \mu e\mathcal{E}(\xi^2 - \eta^2) = 2\mu(\xi + \eta)\alpha_1, \quad (8)$$

where we used that

$$\frac{\xi + \eta}{\xi \eta} = \frac{1}{\xi} + \frac{1}{\eta}, \quad (\xi + \eta)(\xi - \eta) = \xi^2 - \eta^2. \quad (9)$$

The reason for using parabolic coordinates now becomes clear. The Hamilton–Jacobi equation [\(8\)](#) is *separable* in these coordinates.

³ For a detailed explanation of the rationale behind this recipe, see, e.g., [Goldstein et al. \(2002, Chapter 10\)](#) or [Corben & Stehle \(1994, Chapter 11\)](#).

Download English Version:

<https://daneshyari.com/en/article/1161472>

Download Persian Version:

<https://daneshyari.com/article/1161472>

[Daneshyari.com](https://daneshyari.com)