Classical motion of an electron in an electric-dipole field. I. Finite dipole case

Classical motion of an electron in an electric-dipole field. I. Finite dipole case†

J. E. TURNER‡ and K. FOX§‖

‡ Health Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A.
§ Physics Department, The University of Tennessee, Knoxville, and Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A.

Abstract. The classical motion of an electron in the field of a finite electric-dipole is analysed in terms of Hamilton–Jacobi theory. It is shown that a bound state exists for an arbitrarily small dipole moment.

1. Introduction

Because of recent interest in the quantum-mechanical bound states of an electron moving in the field of a finite electric dipole (Wallis *et al.* 1960, Fox and Turner 1966 a, b, Mittleman and Myerscough 1966, Turner and Fox 1966, Lévy-Leblond 1967, Brown and Roberts 1967, Crawford and Dalgarno 1967, Coulson and Walmsley 1967, Crawford 1967, Fox 1967), we wish to present our analysis of the classical problem (Turner and Fox 1965). This analysis gives insight into both quantum and classical aspects of the problem. It shows specifically how, in contrast with the quantum-mechanical result that a minimum dipole moment (1.625×10^{-18} e.s.u. cm) is required to bind an electron, binding occurs classically for an arbitrarily small dipole moment.

2. Hamilton–Jacobi equation

In figure 1 we represent an electron of charge $-e$ in the vicinity of a dipole, centred at the origin O of coordinates, with stationary charges $+q$ and $-q$, comprising the dipole,
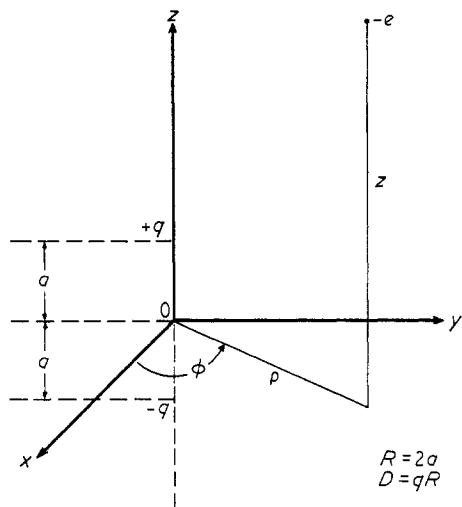

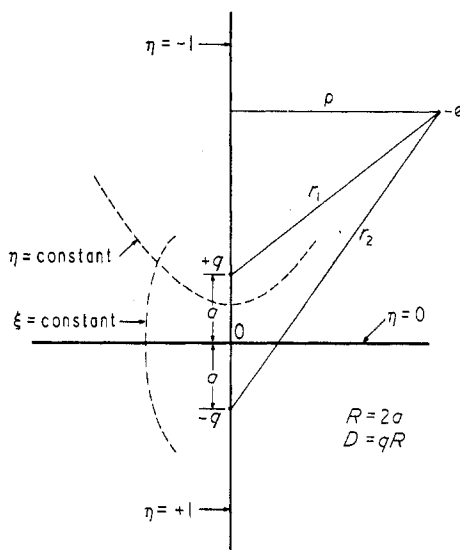Figure 1. Cylindrical coordinate reference system. The dipole moment is $D = 2qa = qR$.

Figure 2. Elliptic–hyperbolic coordinate reference system. The dipole moment is $D = 2qa = qR$.

‖ Now at Jet Propulsion Laboratory, Pasadena, California, U.S.A.

located at the positions $z = +a$ and $z = -a$. The magnitude of the dipole moment is $D = 2qa = qR$. The cylindrical coordinates (ρ, ϕ, z) of the electron are given in terms of its Cartesian coordinates (x, y, z) by the relations $x = \rho \cos \phi$, $y = \rho \sin \phi$, and $z = z$. As shown explicitly below, the angular momentum of the electron about the z axis is constant, and so only two action variables are non-trivial.

In figure 2 we define elliptic–hyperbolic coordinates (ξ, η):

$$\xi = \frac{r_1 + r_2}{R} \qquad (1 \leqslant \xi \leqslant \infty)$$

$$\eta = \frac{r_1 - r_2}{R} \qquad (-1 \leqslant \eta \leqslant 1) \tag{1}$$

where r_1 and r_2 are the distances of the electron from the charges $+q$ and $-q$. In three dimensions, surfaces of constant ξ and η are independent of the azimuthal angle ϕ and thus define ellipsoids and hyperboloids of revolution about the z axis.

The potential energy of the electron is

$$V = qe\left(\frac{1}{r_2} - \frac{1}{r_1}\right). \tag{2}$$

From equation (1) we have

$$r_1 = \tfrac{1}{2}R(\xi + \eta)$$

$$r_2 = \tfrac{1}{2}R(\xi - \eta) \tag{3}$$

and so the potential energy is

$$V = \frac{4qe\eta}{R(\xi^2 - \eta^2)}. \tag{4}$$

In cylindrical coordinates the kinetic energy of the electron is

$$T = \tfrac{1}{2}m(\dot{\rho}^2 + \rho^2\dot{\phi}^2 + \dot{z}^2) \tag{5}$$

where m is the mass of the electron and the dots denote differentiation with respect to time. From the geometry in figure 2 and from equation (3) we may write the equations relating (ρ, z) and (ξ, η):

$$r_1^2 = \rho^2 + (z - a)^2 = a^2(\xi + \eta)^2$$

$$r_2^2 = \rho^2 + (z + a)^2 = a^2(\xi - \eta)^2. \tag{6}$$

Solving for ρ and z in terms of ξ and η and performing the time differentiations, we obtain from equation (5)

$$T = \tfrac{1}{2}ma^2\left\{(\xi^2 - \eta^2)\left(\frac{\dot{\xi}^2}{\xi^2 - 1} + \frac{\dot{\eta}^2}{1 - \eta^2}\right) + (\xi^2 - 1)(1 - \eta^2)\dot{\phi}^2\right\}. \tag{7}$$

The momenta conjugate to the coordinates (ξ, η, ϕ) are defined by the following partial derivatives:

$$p_\xi = \frac{\partial T}{\partial \dot{\xi}} = ma^2(\xi^2 - \eta^2)\frac{\dot{\xi}}{\xi^2 - 1}$$

$$p_\eta = \frac{\partial T}{\partial \dot{\eta}} = ma^2(\xi^2 - \eta^2)\frac{\dot{\eta}}{1 - \eta^2} \tag{8}$$

$$p_\phi = \frac{\partial T}{\partial \dot{\phi}} = ma^2(\xi^2 - 1)(1 - \eta^2)\dot{\phi}.$$

Writing the kinetic energy in terms of these conjugate momenta gives for the Hamiltonian, $H = T + V$,

$$H = \frac{1}{\xi^2 - \eta^2}\left[\frac{1}{2ma^2}\left\{(\xi^2 - 1)p_\xi{}^2 + (1 - \eta^2)p_\eta{}^2 + \left(\frac{1}{\xi^2 - 1} + \frac{1}{1 - \eta^2}\right)p_\phi{}^2\right\} + \frac{2qe\eta}{a}\right]. \tag{9}$$

This expression is consistent with that given for the hydrogen ion molecule H_2^+, for which both electric charges on the z axis in figure 1 are positive (Born 1960). Hamilton's canonical equation $\dot{p}_\phi = -\partial H/\partial \phi$ implies at once from equation (9) that p_ϕ is a constant of the motion since ϕ does not appear explicitly in the Hamiltonian. We are left, therefore, with determining the properties of the motion in terms of ξ and η.

The Hamilton–Jacobi equation is obtained from equation (9) by writing E in place of H for the total energy and $\partial W/\partial \xi$ and $\partial W/\partial \eta$ in place of the momenta p_ξ and p_η (Goldstein 1950). The quantity W, which is Hamilton's characteristic function, generates a canonical transformation from (ξ, η) and their conjugate momenta (p_ξ, p_η) to new variables for which all the momenta are constants of the motion. We treat W as a function of ξ, η and the new conjugate momenta. The Hamilton–Jacobi equation is thus

$$\left\{\frac{\xi^2-1}{2ma^2}\left(\frac{\partial W}{\partial \xi}\right)^2 + \frac{p_\phi^2}{2ma^2}\frac{1}{\xi^2-1} - E\xi^2\right\} + \left\{\frac{1-\eta^2}{2ma^2}\left(\frac{\partial W}{\partial \eta}\right)^2 + \frac{p_\phi^2}{2ma^2}\frac{1}{1-\eta^2} + E\eta^2 + \frac{2qe\eta}{a}\right\} = 0. \quad (10)$$

We assume that W is a sum of two functions, $W = W_\xi(\xi) + W_\eta(\eta)$, where W_ξ and $W\eta$ depend only upon the single coordinate shown (and the new momenta). The first term in curly brackets in equation (10) then depends only on the coordinate ξ and the second term only on η. Equation (10) can then be valid for all values of the independent variables (ξ, η) only if the two bracketed terms are constant. Denoting the values of these constants by $\pm K$, we obtain

$$\left(\frac{\partial W}{\partial \xi}\right)^2 = \frac{2ma^2}{\xi^2-1}\left(K - \frac{p_\phi^2}{2ma^2}\frac{1}{\xi^2-1} + E\xi^2\right)$$

$$\left(\frac{\partial W}{\partial \eta}\right)^2 = \frac{2ma^2}{1-\eta^2}\left(-K - \frac{p_\phi^2}{2ma^2}\frac{1}{1-\eta^2} - E\eta^2 - \frac{2qe\eta}{a}\right). \quad (11)$$

It follows that

$$p_\xi = \frac{\partial W}{\partial \xi} = \frac{(-2ma^2E)^{1/2}}{\xi^2-1}(-\xi^4 + C\xi^2 - A)^{1/2}$$

$$p_\eta = \frac{\partial W}{\partial \eta} = \frac{(-2ma^2E)^{1/2}}{1-\eta^2}(-\eta^4 + B\eta^3 + C\eta^2 - B\eta - A)^{1/2} \quad (12)$$

where the quantities A, B, and C are given by

$$A = -\frac{K}{E} - \frac{p_\phi^2}{2ma^2E}$$

$$B = -\frac{2qe}{aE} = -\frac{De}{a^2E} \quad (13)$$

$$C = 1 - \frac{K}{E}$$

and satisfy the identity

$$A + 1 - C = -\frac{p_\phi^2}{2ma^2E}. \quad (14)$$

3. Analysis of the motion

The motion of the electron takes place in ranges of values of ξ and η for which the momenta in equation (12) are real. For bound states of the electron in the field of the dipole, $E < 0$ and hence the polynomials in equation (12) cannot be negative. That is

$$F(\xi) \equiv -\xi^4 + C\xi^2 - A \geq 0$$
$$G(\eta) \equiv -\eta^4 + B\eta^3 + C\eta^2 - B\eta - A \geq 0. \quad (15)$$

The classical motion takes place between the roots of $F(\xi)$ and $G(\eta)$ in regions where the functions are positive.

We first analyse $F(\xi)$. The roots of this function are

$$\xi_1 = \{\tfrac{1}{2}C - \tfrac{1}{2}(C^2 - 4A)^{1/2}\}^{1/2}$$
$$\xi_2 = \{\tfrac{1}{2}C + \tfrac{1}{2}(C^2 - 4A)^{1/2}\}^{1/2}. \tag{16}$$

We see that, for real ξ_1 and ξ_2, we must require that $C > 0$ and $C^2 \geqslant 4A$. From equation (13) the condition $C^2 \geqslant 4A$ can be expressed as

$$\frac{p_\phi^2}{-2ma^2E} \leqslant \frac{1}{4}\left(1 + \frac{K}{E}\right)^2. \tag{17}$$

Since $\xi \geqslant 1$ by our definition of coordinates (equation (1)), we require that $F(\xi)$ have roots not smaller than unity. This requires that

$$\xi_1{}^2 = \tfrac{1}{2}\{C - (C^2 - 4A)^{1/2}\} \geqslant 1 \tag{18}$$

or that

$$C \geqslant 2 + (C^2 - 4A)^{1/2} \geqslant 2. \tag{19}$$

Since $C \equiv 1 - K/E$, equation (19) implies that $-K/E \geqslant 1$; in addition, equation (13) implies that $A \geqslant 1$. If we carry equation (19) further, we find that $A + 1 - C \geqslant 0$, as already implied for $E < 0$ by equation (14).

The extrema of $F(\xi)$ are obtained by solving

$$\frac{dF}{d\xi} = -4\xi^3 + 2C\xi = 0 \tag{20}$$

which has the roots $\xi = 0$, $\pm(\tfrac{1}{2}C)^{1/2}$. The minimum value of $F(\xi)$ occurs at $\xi = 0$ since $d^2F/d\xi^2 = 2C > 0$ at this point; $F(0) = -A \leqslant -1$. The maximum value of $F(\xi)$ is $F\{\pm(\tfrac{1}{2}C)^{1/2}\} = (\tfrac{1}{4}C^2) - A \geqslant 0$.
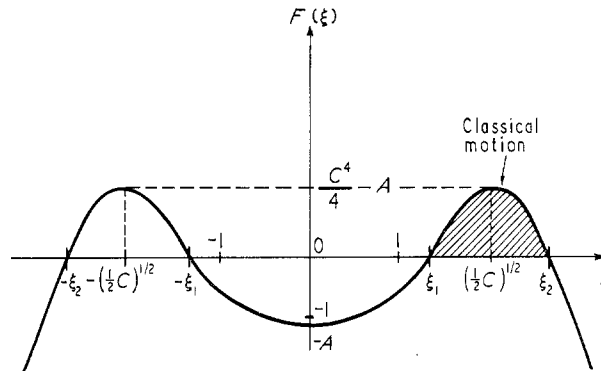

Figure 3. Analysis of $F(\xi)$. The classical motion of an electron in the field of a dipole takes place in the shaded interval.

The form of $F(\xi)$ is illustrated in figure 3 for a case of physically allowed motion. The function is symmetric and $F(\xi) \to -\infty$ as $\xi \to \pm\infty$. The classical motion takes place in the range $\xi_1 \leqslant \xi \leqslant \xi_2$, in which $F(\xi) \geqslant 0$, as indicated by the shaded region in this figure.

For small binding energies the roots ξ_1 and ξ_2 have a simple form. Writing

$$(C^2 - 4A)^{1/2} = \left\{\left(1 - \frac{K}{E}\right)^2 + 4\left(\frac{K}{E} + \frac{p_\phi^2}{2ma^2E}\right)\right\}^{1/2} \tag{21}$$

we obtain, for small E,

$$(C^2 - 4A)^{1/2} \simeq -1 - \frac{K}{E} - \frac{p_\phi{}^2}{ma^2 K}. \tag{22}$$

To this order, the roots are

$$\xi_1 \simeq \left(1 + \frac{p_\phi{}^2}{2ma^2 K}\right)^{1/2}$$

$$\xi_2 \simeq \left(-\frac{K}{E} - \frac{p_\phi{}^2}{2ma^2 K}\right)^{1/2}. \tag{23}$$

As $E \to 0$, $\xi_2 \to \infty$ and so the electron orbit extends to great distances.

The function $G(\eta)$ in equation (15) is the sum of an even and an odd function:

$$G(\eta) = G_E(\eta) + G_O(\eta) \tag{24}$$

with

$$G_E(\eta) = -\eta^4 + C\eta^2 - A$$

$$G_O(\eta) = B\eta(\eta^2 - 1). \tag{25}$$

The function G_E, which is shown as one of the broken curves in figure 4, is identical with the function F, above, and hence has roots at $\eta = \pm\xi_1$ and $\eta = \pm\xi_2$. The function $G_O(\eta)$
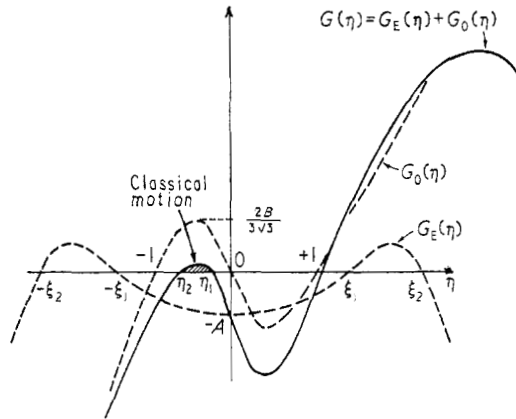

Figure 4. Analysis of $G(\eta)$. The classical motion of an electron in the field of a dipole takes place in the shaded interval.
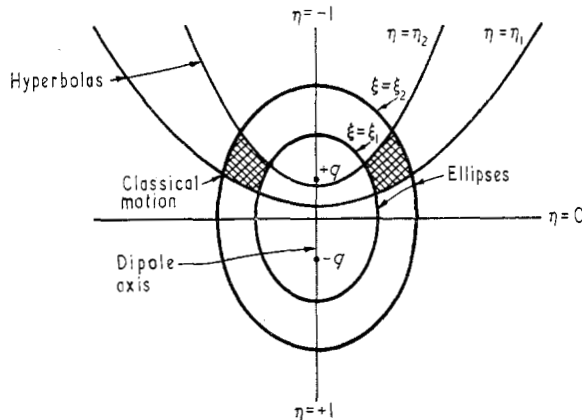

Figure 5. Three-dimensional region of classically allowed orbits contained in the volume generated by revolution of the cross-hatched area about the dipole axis.

has roots at $\eta = 0, \pm 1$. The slope of $G_0(\eta)$ at the origin is $-B$, which by equation (13) is negative for $E < 0$. The extrema of $G_0(\eta)$ occur at $\eta = \pm 1/\sqrt{3}$; $G_0(-1/\sqrt{3}) = +2B/3\sqrt{3}$ is a maximum, and $G_0(+1/\sqrt{3}) = -2B/3\sqrt{3}$ is a minimum. As $\eta \to \pm \infty$, $G_0 \to \pm \infty$. The shape of the function $G_0(\eta)$ is shown by the other broken curve in figure 4. The sum $G(\eta)$, shown by the full curve, can always be made positive in some interval of the region $-1 \leqslant \eta < 0$ by making B large enough. (The roots of $G(\eta)$ in this region are η_1 and η_2.) We see from equation (13) that, for a fixed value of dipole moment, B can be made arbitrarily large if the binding energy $-E$ is taken arbitrarily small.

The allowed classical bound-state orbits lie in a volume defined in three dimensions by rotating the cross-hatched area in figure 5 about the dipole axis. Every orbit is contained in the upper half-space with $1 \leqslant \xi_1 \leqslant \xi \leqslant \xi_2 < \infty$ and $-1 \leqslant \eta_2 \leqslant \eta \leqslant \eta_1 < 0$; the electron cannot enter the lower half-space ($\eta \geqslant 0$).

4. Conclusion

We have shown that a bound state exists for any non-zero value of dipole moment D since, in classical mechanics, the binding energy of the electron is a constant of the motion which can be made as close to zero as desired by a suitable choice of initial conditions. Quantum mechanically, however, it is known that binding of an electron occurs only when $D \geqslant 1 \cdot 625 \times 10^{-18}$ e.s.u. cm.

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