Classical motion of an electron in an electric-dipole field II. Point dipole case

1968 J. Phys. A: Gen. Phys. 1 124

(http://iopscience.iop.org/0022-3689/1/1/317)

J. PHYS. A (PROC. PHYS. SOC.), 1968, SER. 2, VOL. 1. PRINTED IN GREAT BRITAIN

Classical motion of an electron in an electric-dipole field II. Point dipole case†

K. FOX‡
Physics Department, The University of Tennessee, Knoxville, and Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A.

MS. received 11*th September* 1967

Abstract. The classical motion of an electron in the field of a point electric dipole is analysed. It is shown that the only motion for which the distance r from the dipole to the electron does not either increase without limit or decrease to and remain at zero is that for which r is constant and the total energy E is zero. A necessary condition for such bound motion is $D > 3\sqrt{3}p_\phi^2/4me$, where D is the dipole moment, p_ϕ is the component of angular momentum along the dipole axis, and m and e are the electronic mass and charge. It follows that any point dipole can bind an electron classically.

1. Introduction

Recently the classical motion of an electron in the field of a *finite* electric dipole was investigated, especially with a view towards understanding the bound states of the system (Turner and Fox 1965, 1968). In the present work we give a detailed solution for the classical motion of an electron in a *point* electric-dipole field. This problem is of intrinsic interest in classical dynamics. Furthermore, we may obtain some insight into the meaning of bound states in the quantum-mechanical problem (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).

2. Lagrange's equations

The dipole of moment D is oriented along the z axis, is centred at the origin, and has its positive pole in the upper hemisphere. The potential energy of an electron moving in the field of this dipole is $V = -eDr^{-2}\cos\theta$; r, θ, and ϕ are the spherical polar coordinates, and e and m are the electronic charge and mass. (V may be thought of as the limit of the potential energy of an electron moving in the field of a finite dipole, oriented as described in the first sentence, as the extent of the dipole goes to zero with the product of extent and dipole charge remaining finite.)

The Lagrangian for this system is

$$L = T - V = \tfrac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\,\dot{\phi}^2) + eDr^{-2}\cos\theta. \tag{1}$$

Lagrange's equations of motion are

$$\frac{d(m\dot{r})}{dt} - (mr\dot{\theta}^2 + mr\sin^2\theta\,\dot{\phi}^2 - 2eDr^{-3}\cos\theta) = 0 \tag{2}$$

$$\frac{d(mr^2\dot{\theta})}{dt} - (mr^2\sin\theta\cos\theta\,\dot{\phi}^2 - eDr^{-2}\sin\theta) = 0 \tag{3}$$

$$\frac{d(mr^2\sin^2\theta\,\dot{\phi})}{dt} = 0. \tag{4}$$

Equation (4) yields a constant of the motion $p_\phi = mr^2\sin^2\theta\,\dot{\phi}$, the component of angular

† Research sponsored in part by the U.S. Atomic Energy Commission under contract with Union Carbide Corporation.

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

momentum along the dipole axis. Since the force is non-central, the total angular momentum is not a constant of the motion. The constant energy is

$$E = T+V = \tfrac{1}{2}m(\dot{r}^2+r^2\dot{\theta}^2+r^2\sin^2\theta\,\dot{\phi}^2)-eDr^{-2}\cos\theta. \tag{5}$$

That $dE/dt = 0$ may be verified directly from Lagrange's equations.

To solve the dynamical problem, we first multiply equation (2) by r and add that to twice equation (5) to obtain

$$m(r\ddot{r}+\dot{r}^2) = 2E. \tag{6}$$

(In a similar way, the radial equation (6) is obtained for any potential of the form $V = f(\theta, \phi)/r^2$.) This is integrated easily to give

$$\dot{r}(t) = \left(\frac{2E}{m}t+r_0v_0\right)\frac{1}{r(t)} \tag{7}$$

and

$$r(t) = \left(\frac{2E}{m}t^2+2r_0v_0t+r_0{}^2\right)^{1/2} \tag{8}$$

where $r_0 = r(0)$ and $v_0 = \dot{r}(0)$.

Next, we analyse $r(t)$ and $\dot{r}(t)$ for all possible ranges of energy E and initial radial velocity v_0.

3. Analysis of the motion

3.1. *Case* 1. $E < 0$.

(i) $v_0 < 0$. From equation (7) it follows that $\dot{r} < 0$ for all time. Thus r decreases to zero at time $t = (\tfrac{1}{2}mr_0v_0/E)\{(1-E/\tfrac{1}{2}mv_0{}^2)^{1/2}-1\}$, determined from equation (8). There $\dot{r} \to -\infty$.

(ii) $v_0 > 0$. There is a turning point of the motion which occurs at $t = -\tfrac{1}{2}mr_0v_0/E$. At that time $r = r_0(1-\tfrac{1}{2}mv_0{}^2/E)^{1/2}$. After the electron reaches the turning point it heads back towards the dipole and reaches the origin at $t = (-\tfrac{1}{2}mr_0v_0/E)\{1+(1-E/\tfrac{1}{2}mv_0{}^2)^{1/2}\}$. There $\dot{r} \to -\infty$.

(iii) $v_0 = 0$. Thus r decreases to zero at $t = r_0(-2E/m)^{-1/2}$. There $\dot{r} \to -\infty$.

To summarize for $E < 0$: No matter what the initial conditions, the electron eventually goes to and remains at $r = 0$ with $\dot{r} \to -\infty$. That this result occurs for any value of p_ϕ can be understood by assuming $\dot{\phi} \to \infty$ as $r \to 0$. In contrast, for the $1/r$ potential the result $r \to 0$ and $\dot{r} \to -\infty$ occurs only for $p_\phi = 0$. The present result for the $1/r^2$ dependence is analogous to the quantum-mechanical case of a sufficiently attractive $1/r^2$ potential, in which the particle is in an infinitesimally small region about $r = 0$, corresponding to $E \to -\infty$ (the phenomenon of 'fall to the centre' described by Landau and Lifshitz (1965)).

3.2. *Case* 2. $E > 0$.

(i) $v_0 < 0$. There is a turning point at $t = -\tfrac{1}{2}mr_0v_0/E$; $r = r_0(1-\tfrac{1}{2}mv_0{}^2/E)^{1/2}$. However, we can also calculate that the electron reaches $r = 0$ at

$$t = \frac{-\tfrac{1}{2}mr_0}{E}v_0\left\{1-\left(1-\frac{E}{\tfrac{1}{2}mv_0{}^2}\right)^{1/2}\right\}.$$

We must distinguish between the possibilities $E >, <,$ or $= \tfrac{1}{2}mv_0{}^2$.

(*a*) $E > \tfrac{1}{2}mv_0{}^2$. The electron reaches the turning point at $r > 0$. Afterwards $\dot{r} > 0$, and $r \to +\infty$ and $\dot{r} \to (2E/m)^{1/2}$.

(*b*) $E < \tfrac{1}{2}mv_0{}^2$. The electron reaches the origin. There $\dot{r} \to -\infty$.

(*c*) $E = \tfrac{1}{2}mv_0{}^2$. The electron reaches the origin. There $\dot{r} = v_0$ (actually $\dot{r} = v_0$ for all t), or $\dot{r} = -(2E/m)^{1/2}$. The electron does not turn back from the origin.

(ii) $v_0 > 0$. From equation (7), $\dot{r} > 0$ for all time. The electron travels outward with $r \to +\infty$ monotonically; $\dot{r} \to (2E/m)^{1/2}$.

(iii) $v_0 = 0$. The electron travels outward with $r \to +\infty$ monotonically; $\dot{r} \to (2E/m)^{1/2}$.

To summarize for $E > 0$; depending on the initial conditions, the electron either goes to the origin and remains there with $\dot{r} \to -\infty$ or $\dot{r} \to -(2E/m)^{1/2}$, or it goes to $+\infty$ with $\dot{r} = (2E/m)^{1/2}$.

3.3. *Case* 3. $E = 0$.

(i) $v_0 < 0$. From equation (7), $\dot{r} < 0$ for all time. Equation (8) implies that r goes monotonically to zero in a time $t = -\frac{1}{2}r_0/v_0$. There $\dot{r} \to -\infty$.

(ii) $v_0 > 0$. Here $\dot{r} > 0$ for all time; r goes monotonically to $+\infty$, and $\dot{r} \to 0$.

(iii) $v_0 = 0$. In this case $r = r_0$ and $\dot{r} = 0$ for all time. Thus the electron moves on a sphere of radius r_0, with centre at the origin where the point dipole is located. We treat this case in detail in the next section.

4. Bound states

The only instance of physically reasonable bound-state motion has been shown to take place for $E = v_0 = 0$, leading to $r = r_0 =$ constant. We now analyse the angular motion on the sphere.

From equation (5) with $E = 0$, $\dot{r} = 0$, and $p_\phi = mr^2 \sin^2\theta\,\dot{\phi}$, we obtain

$$\tfrac{1}{2}mr^2\dot{\theta}^2 + p_\phi{}^2(2mr^2\sin^2\theta)^{-1} - eDr^{-2}\cos\theta = 0. \tag{9}$$

With the substitution $x = \cos\theta$, equation (9) can be rewritten in the form

$$\dot{x}^2 = 2eD(mr^4)^{-1}(-x^3+x-k) \tag{10}$$

where

$$k = \tfrac{1}{2}p_\phi{}^2(meD)^{-1}. \tag{11}$$

Since increasing θ corresponds to decreasing x, we take the negative square root of equation (10) to obtain

$$t = \int_0^t dt = -\left(\frac{mr^4}{2eD}\right)^{1/2}\int_{x_0}^{x} dx(-x^3+x-k)^{1/2}. \tag{12}$$

Although equation (12) involves an elliptic integral, it is nevertheless possible in principle to obtain $x(t)$.

Thus one can obtain $\theta(t)$, and from $p_\phi = mr^2\sin^2\theta\,\dot{\phi}$ is follows that

$$\phi(t) = \frac{p_\phi}{mr^2}\int_0^t \frac{dt}{\sin^2\theta}. \tag{13}$$

The dynamics of the bound-state motion has been reduced to quadratures. It is still interesting to examine equation (12) for the θ motion in detail.

In order for real solutions to exist, the polynomial $y(x) = -x^3+x-k$ must be positive for some x in the interval from -1 to $+1$. Now $y(+\infty) = -\infty$, $y(-\infty) = +\infty$ and $y(0) = y(\pm 1) = -k \leqslant 0$. The extrema of $y(x)$ occur at $x = \pm 1/\sqrt{3}$. The minimum value is $y(-1/\sqrt{3}) = -k-2/3\sqrt{3}$; the maximum value is $y(+1/\sqrt{3}) = -k+2/3\sqrt{3}$. Clearly $y(x)$ is negative for $-1 < x < 0$. In order for $y(x)$ to be positive in some interval of $0 < x < 1$, the maximum must be positive, i.e. $k < 2/3\sqrt{3}$. This situation is shown in figure 1, for $k = 0{\cdot}3$.

From the definition, equation (11), the condition on k can be expressed as

$$D > \frac{3\sqrt{3}p_\phi{}^2}{4me}. \tag{14}$$

Once p_ϕ is specified by the initial conditions, equation (14) is a strong condition requiring a minimum dipole moment for binding. Of course, for $p_\phi = 0$ any non-zero dipole moment will satisfy the condition. Turning the argument around, we may say that for a given dipole moment it is always possible to achieve bound-state motion, since initial conditions can always be chosen so that equation (14) is satisfied. This is true for the finite-dipole problem also (Turner and Fox 1965, 1968). (If p_ϕ is quantized in an appropriate way, equation (14) yields the minimum dipole moments required for binding in the ground state and in certain excited states of the quantum-mechanical motion of an electron about a finite or point dipole (Fox 1967).)

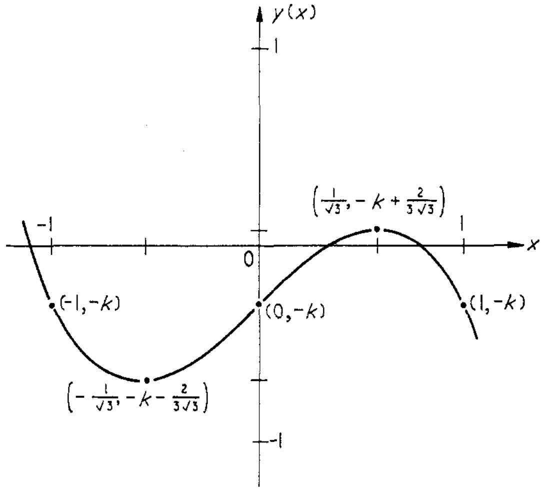

Figure 1. A plot of the function $y(x) = -x^3+x-k$, for $k = 0{\cdot}3$.

The turning points in the θ motion are given by $\dot{\theta} = 0$, or $\dot{x} = 0$. The roots of the polynomial $y(x) = -x^3+x-k$ occur for $0 \leqslant x \leqslant 1$, as indicated in figure 1. Thus the electron moves only in the upper hemisphere, as in the classical finite-dipole problem.

Acknowledgments

The author wishes to thank Dr. J. E. Turner for a critical reading of the manuscript and for many helpful comments.

References

Brown, W. B., and Roberts, R. E., 1967, *J. Chem. Phys.*, **46,** 2006–7.
Coulson, C. A., and Walmsley, M., 1967, *Proc. Phys. Soc.*, **91,** 31–2.
Crawford, O. H., 1967, *Proc. Phys. Soc.*, **91,** 279–84.
Crawford, O. H., and Dalgarno, A., 1967, *Chem. Phys. Lett.*, **1,** 23.
Fox, K., 1967, *Phys. Lett.*, **25A,** 345–6.
Fox, K., and Turner, J. E., 1966 a, *Am. J. Phys.*, **34,** 606–10.
—— 1966 b, *J. Chem. Phys.*, **45,** 1142–4.
Landau, L. D., and Lifshitz, E. M., 1965, *Quantum Mechanics, Non-Relativistic Theory,* 2nd edn (Reading, Mass.: Addison-Wesley), pp. 113–6.
Lévy-Leblond, J. M., 1967, *Phys. Rev.*, **153,** 1–4.
Mittleman, M. H., and Myerscough, V. P., 1966, *Phys. Lett.*, **23,** 545–6.
Turner, J. E., and Fox, K., 1965, *Oak Ridge National Laboratory Rep.* No. ORNL-3895.
—— 1966, *Phys. Lett.*, **23,** 547–9.
—— 1968, *J. Phys.* A (*Proc. Phys. Soc.*), [2], **1,** 118–23.
Wallis, R. F., Herman, R., and Milnes, H. W., 1960, *J. Molec. Spectrosc.*, **4,** 51–74.