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ION MOTION IN ELECTROSTATIC DIPOLE FIELDS*

by

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CHAPTER I

INTRODUCTION

The motion of a charged particle in an anisotropic potential field presents interesting features, such as non-planar scattering. Certain aspects of this motion, eg., the bound state problem and the scattering problem have been investigated both quantum mechanically and to some extent classically. Before taking to our specific problem of the classical unbound motion of an ion in the field of a fixed point electrostatic dipole, we shall give a general background of what has been investigated both quantum mechanically and classically for the general problem of motion of charged particles in the field of an electrostatic dipole.

The interaction between the charge of an electron and the dipole moment of a polar molecule gives rise to a long distance force which significantly modifies the electron scattering process. The cross section for this process has been calculated for the case of a point dipole scatterer by Altshuler[1] in the first Born approximation and exactly by Mittleman and Von Holdt[2]. Since the experimental results for some polar molecules like water do not agree with these theories,Turner[3] has tried to explain this discrepancy by considering the possibility of a temporary capture of the electron with rotational excitation of the molecule. Turner and Fox[4] have calculated by a WKB method, the minimum dipole moment required for the existence of bound states. Papers also have been published about the problem of capture and bound states by Levy-Leblond[5], and

Wallis et al[6]. The cross section for slow electron scattering by a strongly polar molecule has also been calculated recently by Itikawa[7]. A semiclassical theory of capture collisions between ions and polar molecules has also been advanced by Dugan and Magge[8].

Turning to classical treatments, we find very few references. The classical bound states of an electron in the field of a finite dipole have been analyzed by Turner and Fox[9]. Cross and Hershback[10] have studied the problem of classical scattering of an atom from a diatomic rigid rotor due to an anisotropic potential consisting of a Lennard-Jones function multiplied by $[1 + aP_2(\cos\gamma)]$, where a is an asymmetry parameter, γ the angle between the axis of the molecule and the radius vector to the atom, and P_2 the second even Legendre Polynomial. By closely following Whittaker[11], and choosing appropriate coordinates and momenta, they have been able to reduce to seven the number of differential equations of motion for this three body problem. Cross[12] has also derived a method of calculating small angle scattering from an arbitrary anisotropic potential, using either an impulse approximation, or perturbation solution of Hamilton's equations of motion. He has subsequently applied this to ion-dipole scattering, and shown that the differential cross section in some sense approximates that for a spherically symmetric potential given by $\frac{ke}{2r^2}$.

A special case of this analysis has very recently been given by Fox[13], who has kindly supplied us with preprints of his work and that of Fox and Turner[14]. Aspects of the present treatment have been given by Wilkerson[15]. Suchy[16] and Spiegel[17] have separately indicated how one might set up the Hamilton-Jacobi integrals, without carrying out further steps. It turns out that additional insights into the symmetry properties of the motion are required in order to carry through the analysis. Aside from special cases in the books by Loney[18] and Corben and Stehle[19], our extensive literature search has not uncovered any instance of this problem having been previously considered to the extent that one might expect.

The problem seems to us to hold special interest because of the fundamental and simple anisotropy of the potential, i.e. a field having one attractive and one repulsive hemisphere with a vanishingly small radial component at large distances. One intuitively expects the features of this motion to be in a sense prototypical of more general and complicated motions in anisotropic fields.

Thanks to the anisotropic nature of the interaction between the ion and the dipole, the trajectory of the ion will not be confined to a plane, except in special circumstances. In the following pages we have developed a formalism, which we believe represents the first analytical approach to this complex problem of the classical trajectory of an ion in the field of an electrostatic dipole. With this formalism, the entire trajectory of the ion can be traced.

Figure 1 summarizes the coordinates used in our analysis of the problem. The proton with charge $+e$ moves in the field of a fixed point electrostatic dipole. As the potential takes a simple form, when we use spherical coordinates, we represent the position of the ion at the general time t by the spherical coordinates r, θ and ϕ. The dipole moment of strength $\vec{k}$ is aligned along the z axis, as the familiar limiting case of the finite dipole having its positive charge on the positive side of the z axis, and its center coinciding with the origin. The Hamiltonian H for such a system can be written as

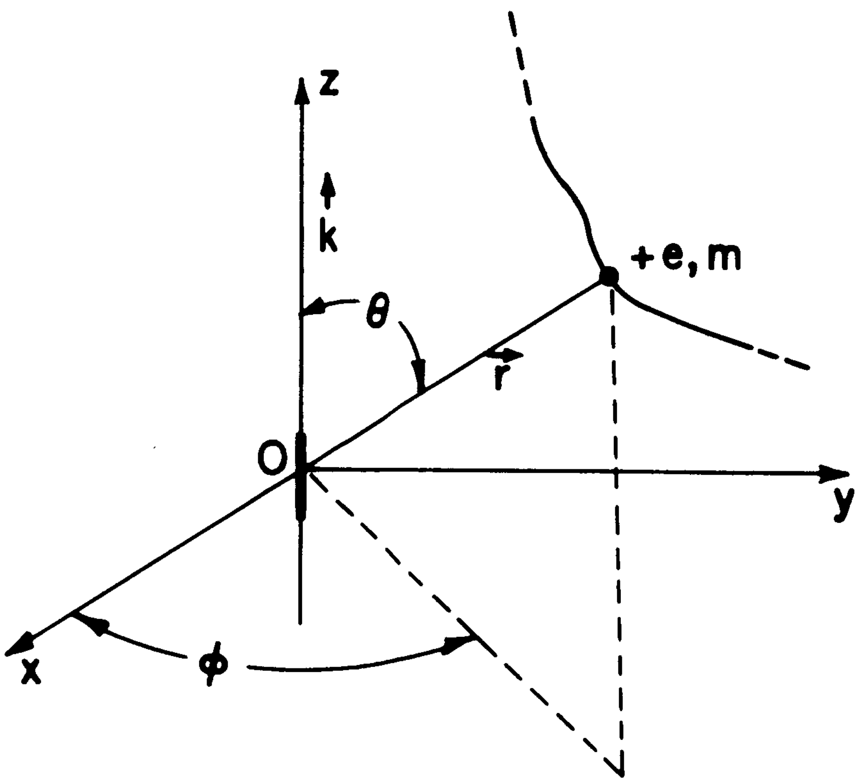

FIGURE I. POSITION OF THE ION IN SPHERICAL COORDINATES.

$$H = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2\sin^2\theta} + \frac{ke\cos\theta}{r^2} \qquad (1.1)$$

where m and e are the mass and charge of the ion respectively.

We are interested in the classical unbound motion of the ion, as this has great significance to the general scattering problem. For a specific problem -- the proton-water molecule interaction -- considering the polar molecule to be fixed in position and orientation seems to be a reasonable approach. This is so, since, for the scattering of sufficiently energetic ions, (energy $E > 100$ electron volts) molecular rotation can be neglected. We believe a complete solution of this restricted problem will prove important in treating the motion of an ion in more general circumstances.

The scheme that we have followed in the presentation of our calculation is as follows: Chapter II deals with the constants of motion and certain aspects of this problem; Chapter III, with the specific case of motion in the meridian plane; Chapter IV, with the general case of non-planar motion; Chapter V, with a few specific calculations of trajectories and a discussion about these trajectories; and Chapter VI, with a summary and critique of the dissertation. Appendices A and B are concerned, respectively, with a review of elliptic functions and an estimation of the ion energy above which the turning of a free dipole (in response to the ion's presence) may be neglected.

CHAPTER II

UNIQUE ASPECTS OF THE PROBLEM

In this Chapter we introduce the problem of ion motion in the field of a fixed point electric dipole and discuss certain unique features of this problem.

The Hamiltonian for the system is

$$H = \frac{1}{2m} \left[p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2\theta} \right] + \frac{ke \cos\theta}{r^2}$$

where m is the mass of the ion, e its charge, k the dipole moment of the center of force, (e.g., a polar molecule fixed in position and orientation) and r, θ, and ϕ are the spherical coordinates of the ion at the general time t, whose initial position at time $t = o$ is r_o, θ_o and ϕ_o.

It is clear that p_ϕ is a constant, since the Hamiltonian is cyclic in ϕ. We can group terms in the Hamiltonian by writing

$$H = \frac{p_r^2}{2m} + \frac{1}{r^2} f; \quad f = \frac{p_\theta^2}{2m} + \frac{p_\phi^2}{2m \sin^2\theta} + ke \cos\theta \ .$$

Hamilton's equations for the radial coordinate and momentum are

$$\frac{\partial H}{\partial p_r} = \dot{r} = \frac{p_r}{m} \ ; \quad - \frac{\partial H}{\partial r} = \dot{p}_r = + \frac{2}{r^3} f \ . \tag{2.1}$$

Therefore,

$$m\ddot{r} = \dot{p}_r = \frac{2}{r^3} f \quad .$$

Since all the criteria are met for the Hamiltonian and total energy E to be equal and to be constant, we also know that

$$\left(E - \frac{p_r^2}{2m}\right) r^2 = f \quad . \tag{2.2}$$

Eliminating f between (2.1) and (2.2) one finds

$$m\,(r\ddot{r} + \dot{r}^2) = m\,\frac{d}{dt}\,(r\dot{r}) = 2E \tag{2.3}$$

which is easily integrated twice to give

$$r^2(t) = \frac{2E}{m}\,t^2 + 2\,r_o\,\dot{r}_o t + r_o^{\,2}, \tag{2.4}$$

where r_o and $\dot{r}_o$ are the values of radial coordinate and velocity respectively when $t = 0$. Thus we find the square of the magnitude of the radius vector to the point charge to be simply a quadratic polynomial in time. This is a general feature of potentials of the type $F(\theta,\phi)/r^2$, no matter what the form of $F(\theta,\phi)$; $\cos\theta$ in our present case, or unity for "Cotes' spirals"[20] for example.

Relation (2.2) is remarkable in another respect, in that it clearly shows a separation into radial and angular quantities. For example, by invoking knowledge of the radial coordinate, velocity and momentum, it can be shown that

$$(2mE - p_r^2)\, r^2 = (2mE - p_{r_o}^2)\, r_o^2$$

and hence that another constant of the motion α also exists.

$$\alpha = p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta} + 2mke\cos\theta \; .$$

$$= p_{\theta_o}^2 + \frac{p_{\phi_o}^2}{\sin^2\theta_o} + 2mke\cos\theta_o \; , \qquad (2.5)$$

where $p_\phi = p_{\phi_o}$ also.

Another way of putting it of course is that the Hamilton-Jacobi equation for this problem is at least partly separable, and that α is just the separation constant between the radial and angular parts of the problem. It will be seen that further separation (with θ and ϕ) requires more specific detail in the potential - such as the indicated one $F(\theta,\phi) = \cos\theta$ - and does not allow a complete arbitrariness as to the angular dependence of the potential.

In the case of spherically symmetric potentials, the (total angular momentum)$^2 = p_\theta^2 + \dfrac{p_\phi^2}{\sin^2\theta}$ is conserved. But here it is not conserved. Only the quantity $p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta} + 2mke \cos\theta$ is conserved. As a result, the trajectory in general is not confined to a plane.

The constants of motion are readily seen to be (1) Energy E, (2) $\alpha = p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta} + 2mke\cos\theta$ and (3) the z component, p_ϕ, of the total angular momentum.

A. Transformation of Time Coordinate

Though the expression for $r^2(t)$ given in (2.4) is a very simple and interesting one, its lack of time symmetry presents a small barrier to several interesting conclusions.* This is easily removed by a translation to a new time coordinate τ, such that r is an extremum $(\dot{r} = o)$ when $\tau = o$. By simple calculations on a quadratic form $r^2 = at^2 + bt + c$, one can show that $t = \tau - \frac{b}{a}$, whence the linear term drops out, and we have in this case

$$r^2(\tau) = \frac{2E}{m}\tau^2 + \frac{\alpha}{2mE} \tag{2.6}$$

where

$$\tau = t + \frac{m r_o \dot{r}_o}{2E}$$

*It will be seen in Chapter 4 that this symmetrization is vital in accomplishing the ϕ integration.

and

$$\alpha = r_o^2(2mE - p_{r_o}^2)$$

These relations immediately enable one to identify the **unbounded (i.e., scattering) orbits in terms of the constants** E and α. By a "scattering orbit", one means an orbit reaching out to infinite distance in both time directions. In the (r,τ) plane, we require that (2.6) appear as a hyperbola with focus on the r-axis at time $\tau = o$ $(t = -\frac{m r_o \dot{r}_o}{2E})$. This is shown in Figure 2. The canonical form for discussing (2.6) in this context is

$$\frac{r^2}{\left(\sqrt{\frac{\alpha}{2mE}}\right)^2} - \frac{\tau^2}{\left(\frac{\sqrt{\alpha}}{2E}\right)^2} = 1. \qquad (2.7)$$

from which it is clear that neither α nor E can be negative and still maintain the conditions for a scattering orbit. Fox[13] has discussed the indeterminate case $\alpha = E = o$ giving $r^2 = r_o^2$. For E strictly zero, and α not necessarily zero, the earlier form (2.4) demonstrates an inability of the orbits to reach infinity, either in positive or negative time depending on the sign of $\dot{r}_o$. In any case, it is more fruitful to examine orbits for which $\alpha > o$ and $E > o$ and let these parameters then become small in order to understand the unusual cases of motion. More important, we must deal with the entire classes of solutions for which both α and E are positive, in order to deal with the scattering problem.

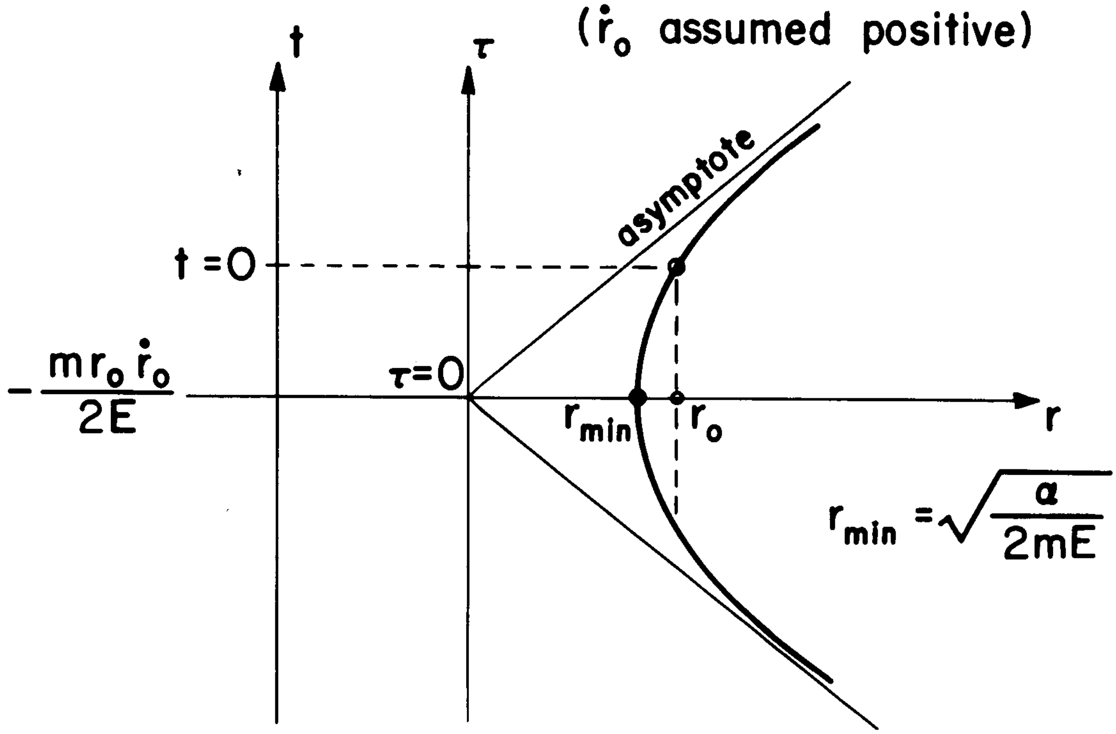

Figure 2. Translation Of The Origin Of Time.

B. Minimum Distance of Approach

From (2.5) we can write

$$\alpha = 2mE\, b_{-\infty}^{2} + 2mek \cos \theta_{-\infty} \tag{2.8}$$

where

$b_{-\infty}$ is the impact parameter

and

$\theta_{-\infty}$ the polar angle θ at time $t = -\infty$.

From (2.6) we also know that

$$\alpha = 2Em\, r^{2}_{min} \quad . \tag{2.9}$$

Therefore,

$$r^{2}_{min} = b_{-\infty}^{2} + \frac{ek}{E} \cos \theta_{-\infty} \ . \tag{2.10}$$

This relation defines the minimum distance, r_{min}, in terms of the initial impact parameter, energy, dipole strength and the angle $\theta_{-\infty}$. From (2.10), we can note the following:

(1) The minimum distance for the repulsive hemisphere, i.e. $o \leqslant \theta < \frac{\pi}{2}$, is always greater than zero, no matter what the impact parameter is.

(2) It increases with increase in impact parameter, or dipole moment k, and decreases with increase in energy.

(3) It is strongly angular dependent, and for a given choice of k, E and $b_{-\infty}$, decreases from a maximum value for $\theta = o^\circ$, to a minimum value for $\theta = 180^\circ$.

C. Turning Points

For the central force there is only one kind of turning point, namely where the radial velocity $\dot{r}$ becomes zero. At this turning point, we have for $w = 1/r$,

$$w = w(o), \quad \left(\frac{dw}{d\theta}\right)_o = o \quad \text{for} \quad \theta = o .$$

By contrast, the dipole problem possesses two types of turning points. These are the radial turning point ($\dot{r} = o$), and the angular turning point for the polar angle θ ($\dot{\theta} = o$). From (2.6), it follows that the radial turning point is reached at zero time, and it corresponds to minimum radial distance.

At the radial turning point, $(\frac{dr}{d\theta})$ is zero and $(\frac{d\theta}{dr})$ is infinite except for $\frac{d\theta}{d\tau} = o$. This can be shown as follows:

Since

$$dr/d\tau = (dr/d\theta)(d\theta/d\tau),$$

it readily follows

$$\left(\frac{dr}{d\theta}\right) = o \quad \text{if} \quad \left(\frac{d\theta}{d\tau}\right) \neq o. \tag{2.11}$$

From the Hamiltonian given in (1.1),

$$p_\theta = mr^2 \frac{d\theta}{d\tau} \quad ,$$

which can be rewritten using (2.6) as

$$p_\theta = (\frac{d\theta}{dr})\ r\ (2\ Emr^2 - \alpha)^{1/2} \tag{2.12}$$

Thus,

$$\frac{d\theta}{dr} = \frac{p_\theta}{r(2Emr^2 - \alpha)^{1/2}} \quad . \tag{2.13}$$

When the radial turning point is reached, $r = r_{min}$, and $(2mEr_{min}^2 - \alpha) = o$; whence $(\frac{d\theta}{dr})$ becomes infinite, provided $p_\theta \neq o$.

For the simple case of motion in the meridian plane i.e., p_ϕ = const = o, the angular turning point can be found by using equation (2.5). Thus,

$$p_\theta = \pm (2mke)^{1/2} (\frac{\alpha}{2mke} - \cos\ \theta)^{1/2}\ ;\ p_\phi = const = o \tag{2.14}$$

so from equation (2.14), we can note that

$$\dot{\theta} = o \quad \text{when} \quad \theta = \cos^{-1} (\frac{\alpha}{2mke}) \tag{2.15}$$

Equation (2.15) defines the angular turning point, and it can be readily seen that no angular turning point exists when $\alpha/2mke > 1$.

For the more general case of non-planar motion, the angular turning points can be found from the relation,

$$p_\theta = \pm\sqrt{2mke}\left\{\frac{\alpha}{2mke} - \frac{p_\phi^2}{\sin^2\theta}\frac{1}{2mke} - \cos\theta\right\}^{1/2} \qquad (2.16)$$

with the substitution $\cos\theta = u$, this reduces to

$$p_\theta = \pm\sqrt{2mke}\ \frac{\left\{u^3 - \frac{\alpha}{2mke}u^2 - u + \frac{\alpha}{2mke} - \frac{p_\phi^2}{2mke}\right\}^{1/2}}{(1-u^2)^{1/2}} \qquad (2.17)$$

which can be factored as

$$p_\theta = \pm\sqrt{2mke}\left\{\frac{(u-u_1)(u-u_2)(u-u_3)}{(1-u^2)}\right\}^{1/2}; \qquad u^2 \neq 1 \quad (2.18)$$

where u_1, u_2 and u_3 are the roots of the cubic polynomial in u. As we shall show in the next Chapter, motion can take place only when the value for u is between u_2 and u_3, the lower two of the three roots. So equation (2.18) enables us to determine the angular turning points, which are defined by the relation

$$\theta_2 = \cos^{-1}(u_2) \quad \text{and} \quad \theta_1 = \cos^{-1}(u_3);\ u_1 > u_2 > u_3$$

We have shown in Chapter 4, that

$$1 > u_2 > u_3 \quad \text{and} \quad -1 < u_3 < u_2 \quad .$$

For p_ϕ = const $\neq$ o, we therefore have two angular turning points. At the angular turning point, from (2.13), it is evident that $(d\theta/dr)$ is zero, and $(dr/d\theta)$ is infinity, except for $(dr/d\tau)$ = o. If the angular and radial turning points are both zero simultaneously, then both $(dr/d\theta)$, and $(d\theta/dr)$ are indeterminate, at the common turning point.

Finally we may add that there is no turning point corresponding to the azimuthal angle ϕ, and this is due to the fact that the dipole potential has no ϕ dependence.

D. The Orbits

We shall now investigate how the differential orbital equation for this anisotropic potential differs from its counterpart in the case of a central potential. For this purpose, we shall consider the simple case of motion with p_ϕ = const = o, which we will discuss in the next Chapter in detail. The advantage of choosing this subset of orbits for the dipole problem is that, being entirely planar, these orbits make the closest approach to the case of central force motion, in which all orbits are planar. Morever, the (r,θ) motion in a meridian plane sees the full anisotropy of the dipole potential, whence we can expect some of the differences from central force motion to emerge the most strikingly. Our inquiry in this section extends to the question of symmetry or asymmetry of spatial orbits under reflection about the apsidal vector (vector from the origin to the radial turning point.)

Writing the Hamiltonian for our problem as

$$H = \frac{p_r^2}{2m} + \frac{1}{2mr^2} \alpha ,$$

one finds from Hamilton's equations for the radial coordinate and momentum,

$$m\ddot{r} - \frac{\alpha}{mr^3} = o \tag{2.19}$$

Since $mr^2(d\theta/d\tau) = \pm (\alpha - 2mke \cos \theta)^{1/2}$, for p_ϕ = constant = o, we write

$$\frac{d}{d\tau} = \pm \frac{(\alpha - 2mke \cos \theta)^{1/2}}{mr^2} \frac{d}{d\theta} \tag{2.20}$$

Therefore,

$$\frac{d^2r}{d\tau^2} = \pm \frac{(\alpha - 2mke \cos \theta)^{1/2}}{mr^2} \frac{d}{d\theta} \left\{ \pm \frac{(\alpha - 2mke \cos \theta)^{1/2}}{mr^2} \frac{dr}{d\theta} \right\}$$

(It may be observed, that though the sign of p_θ may change during motion, this will not affect the second derivative of r with respect to time). Defining $w = 1/r$, we can rewrite this as

$$\frac{d^2r}{d\tau^2} = -\frac{(\alpha - 2mke\cos\theta)^{1/2}}{m^2} w^2 \frac{d}{d\theta}\left\{(\alpha - 2mke\cos\theta)^{1/2}\frac{dw}{d\theta}\right\}$$

Simplifying and substituting into (2.19) yields the $(u - \theta)$ relation in differential form as

$$\left(\frac{\alpha}{2mke} - \cos\theta\right)\frac{d^2w}{d\theta^2} + \frac{\alpha}{2mke}\, w + \frac{\sin\theta}{2}\,\frac{dw}{d\theta} = o \qquad (2.21)$$

This relation indicates that only when θ is zero at the radial turning point, can we reflect the orbit about a vector which will leave it invariant. Since the polar angle θ in our problem is already defined in relation to the dipole axis, the situation of the radial turning point lying precisely <u>on</u> the dipole axis constitutes a special case. So we may conclude, that for the dipole potential, for this sub category i.e., p_ϕ = const = o, we cannot generally reflect the orbit, about the apsidal vector, except in very special situations. On the other hand, we may note that in the case of central force, we can <u>always reflect</u> the orbit about the apsidal vector, and this is because of two reasons (1) the form of the $(u - \theta)$ differential equation and (2) we can arbitrarily make the angle equal to zero, at the turning point.

It is interesting to explore the special situations we have referred to in the previous paragraph. When the radial turning point occurs on the axial line, we can see from (2.21) that the orbit can be reflected about the axial vector.* Similarly it can be shown that if the radial turning point occurs on the negative side of the z-axis, we can reflect the orbit about the negative side.** For a given E and α, there is only one such orbit; i.e., these orbits are uniquely determined by two parameters E and α.

For the case $\alpha/2mek < 1$, there is an interesting possibility, that both the angular and radial turning points may occur simultaneously. As we have shown above, this implies that $dr/d\theta$ becomes indeterminate. For this case, a study of θ as a function of time, (given in Chapter 3) will establish that $\theta(\tau) = \theta(-\tau)$. As we know already that $r(\tau) = r(-\tau)$, it follows that the radial and angular coordinates are independent of the <u>sign of time</u>. It is perhaps reasonable to conclude that the ion may describe some path until it reaches the minimum distance, when both the radial and angular velocities become zero, and then <u>retrace its path</u>. Since we have assumed α to be always positive, this common turning point, if it exists at all, has to be in the repulsive hemisphere. We will explore these cases in greater detail in Chapter III.

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*Note that when θ goes to $-\theta$, the terms $\sin\theta \frac{dw}{d\theta}$, and $\cos\theta \frac{d^2w}{d\theta^2}$ remain unaffected. Also we can redefine measurement of the angle θ, as the right side of the z-axis corresponding to angle θ, from o to π, and the left side from o to $-\pi$. This redefinition is valid, since it does not change the Hamiltonian.

**This can be shown by redefining the z-axis. Now the potential term will be $-\frac{ke\cos\theta}{r^2}$; the constant α will take a new value, but the form of the equation (2.21) will be preserved.

CHAPTER III

MOTION IN THE MERIDIAN PLANE

In this Chapter, we deal with motion in the meridian plane i.e., p_ϕ = const = o. This category will be comparatively simple to understand, and we hopefully expect that one can get valuable insight into certain interesting aspects of this problem, which can afterwards be generalized to cover more general cases. Motion will always take place in the meridian plane, whenever the initial velocity vector and the dipole axis are in the same plane.

A. Evaluation of Integrals for the Case $p_\phi = o$

From the Hamiltonian given in (1.1),

$$p_\theta = mr^2 \frac{d\theta}{d\tau} ,$$

which can be used to write the $(\theta - \tau)$ integral equation as

$$\int_{\theta_o}^{\theta(\tau)} \frac{d\theta}{p_\theta} = \int_o^\tau \frac{d\tau}{mr^2(\tau)} \tag{3.1}$$

we can change the integration variable θ to $u = \cos\theta$ and use (2.16) to rewrite (3.1) as

$$\int_{u_o}^{u_\tau} \frac{\pm du}{(2mke)^{1/2}} \left\{u^3 - \frac{\alpha}{2mke} u^2 - u + \frac{\alpha}{2mke}\right\}^{1/2} = \int_o^\tau \frac{d\tau}{mr^2(\tau)} . \quad (3.2)$$

The negative sign is to be taken when p_θ is initially positive, and the positive sign when p_θ is initially negative. Though p_θ may change sign, during motion, this will not affect the evaluation of the θ integral, and this has been shown in Appendix A.

The cubic polynomial in u can be factored so that

$$f(u) \equiv \left\{u^3 - \frac{\alpha}{2mke} u^2 - u + \frac{\alpha}{2mke}\right\} = (u - \frac{\alpha}{2mke})(u + 1)(u - 1) \quad (3.3)$$

where $\frac{\alpha}{2mke}$, + 1 and - 1 are the roots of $f(u)$. So the $(u - \tau)$ integral equation can finally be written as

$$\pm \int_{u_o}^{u_\tau} \frac{du}{(2mke)^{1/2}} \left\{(u - \frac{\alpha}{2mke})(u - 1)(u + 1)\right\}^{1/2} = \int_o^\tau \frac{d\tau}{2E(\tau^2 + \frac{\alpha}{4E^2})} \quad (3.4)$$

where u_τ and u_o are the cosines of the polar angles θ_τ and θ_o at time τ and o respectively.

All these roots are real, and in <u>descending</u> order may be either $(\alpha/2mke, + 1, - 1)$ or $(1, \alpha/2mke, - 1)$ according as $\alpha/2mke$ is greater than or less than 1. We can adopt a procedure similar to discussions on the general motion of a spherical pendulum[21] and the symmetrical top,[22] for the dipole problem. As mentioned in the last paragraph $f(u)$ has three real zeros $\alpha/2mke$, $+1$ and -1. With the roots arranged in descending order and labelled as u_1, u_2 and u_3, the graph between u and $f(u)$ will look as given in Figure 3. Since $f(u)$ has to be non negative during motion, we conclude that u can take only values between the two roots u_2 and u_3. Thus we see that while for the case $\alpha/2mke > 1$, θ can take all values from o to π, for the case $\alpha/2mke < 1$, θ can take only values from π to $\cos^{-1}(\alpha/2mke)$.

The u integral in (3.4) can be written in a standard form

$$I \equiv \int_{u_o}^{u_\tau} \frac{-du}{(2mke)^{1/2}\left\{f(u)\right\}^{1/2}} = \frac{1}{(2mke)^{1/2}}\left[\int_{u_3}^{u_o} \frac{du}{\left\{f(u)\right\}^{1/2}} - \int_{u_3}^{u_\tau} \frac{du}{\left\{f(u)\right\}^{1/2}}\right] \tag{3.5}$$

The integral I can be evaluated in terms of inverse elliptic functions[23] so we get

$$I = \frac{2}{(u_1 - u_3)^{1/2}} \frac{1}{(2mke)^{1/2}} \left[\mathrm{Sn}^{-1}\left\{\left(\frac{u_o - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\} - \mathrm{Sn}^{-1}\left\{\left(\frac{u_\tau - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\}\right] \tag{3.6}$$

where the notation Sn represents one of the Jacobian elliptic functions; these functions are discussed in Appendix A. Here the arguments of the functions are $\left\{(u_o - u_3)/(u_2 - u_3)\right\}^{1/2}$ and $\left\{(u_\tau - u_3)/(u_2 - u_3)\right\}^{1/2}$ and the functional parameter is $(u_2 - u_3)/(u_1 - u_3)$, commonly denoted by M.

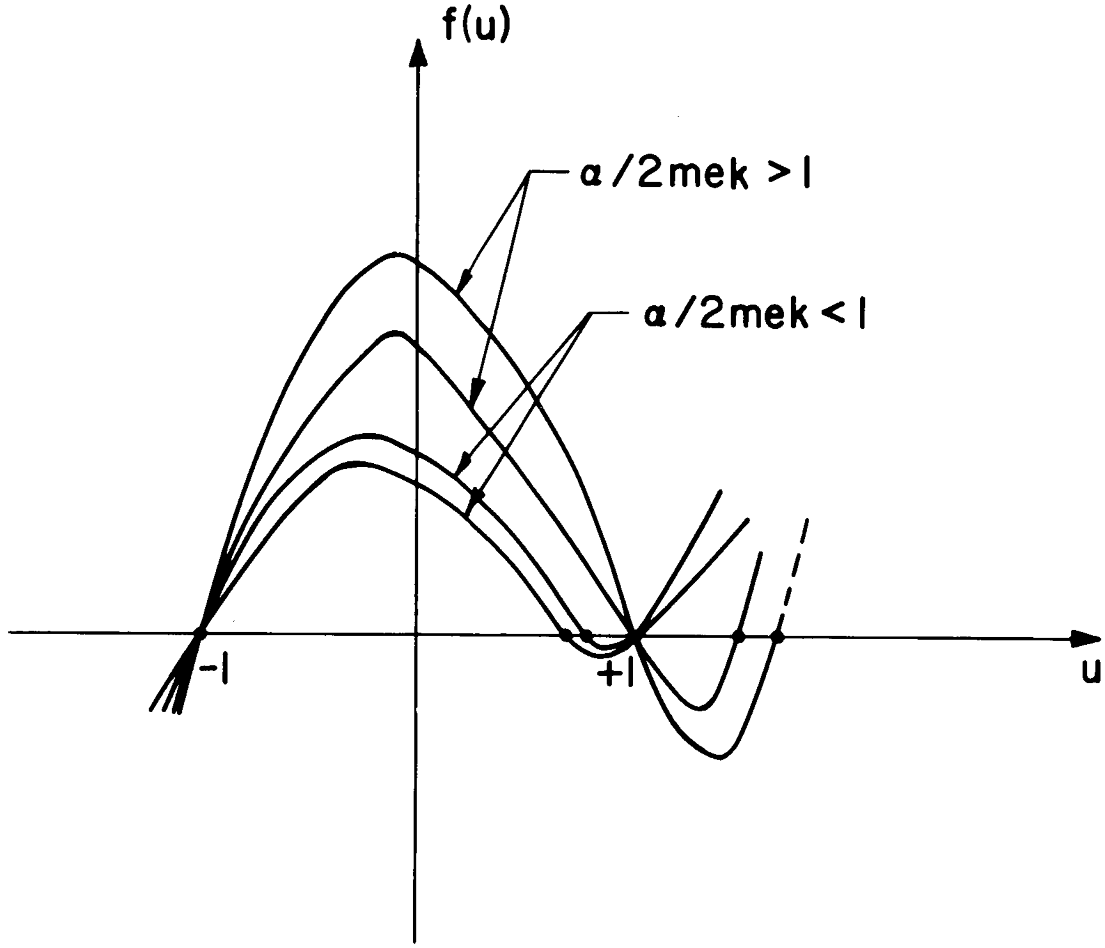


Figure 3. Pictorial Representation Of f(u) For Meridian Plane Motion.

The time integral in (3.4) is

$$\int_o^{\tau} \frac{d\tau}{2E(\tau^2 + \frac{\alpha}{4E^2})} = \frac{1}{\sqrt{\alpha}} \mathrm{Tan}^{-1} \left(\frac{2E}{\sqrt{\alpha}} \tau\right) \tag{3.7}$$

So $(u - \tau)$ integral fully evaluated on both sides gives

$$\mathrm{Sn}^{-1} \left\{ \left(\frac{u_o - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M \right\} - \mathrm{Sn}^{-1} \left\{ \left(\frac{u_{\tau} - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M \right\} = \pm\, c\ \mathrm{Tan}^{-1} \left(\frac{2E}{\sqrt{\alpha}} \tau\right) \tag{3.8}$$

where

$$c = \sqrt{\frac{mke}{2\alpha} (u_1 - u_3)} \quad .$$

The positive sign is when p_θ is initially positive, and the negative sign when p_θ is initially negative.

From (3.8), we can see that the polar angle θ can be expressed as a function of time, provided α is known. The constant α can be calculated from the initial conditions of the problem. Thus we can write, as given in (2.8),

$$\alpha = 2mE\, b_{-\infty}^2 + 2me\, k \cos \theta_{-\infty}$$

where $b_{-\infty}$ is the impact parameter and $\theta_{-\infty}$ is the polar angle θ at time $\tau = -\infty$. This expression enables us to calculate α, provided the impact parameter $b_{-\infty}$ and the polar angle $\theta_{-\infty}$ are known.

Further consequences of our evaluation of the motion for p_ϕ = const = o, require some attention to the magnitude of $\alpha/2mke$ relative to unity.

B. Different Cases of Magnitude of $\alpha/2mke$

Case I. $\alpha/2mke >> 1$.

The roots in descending order are:

$$u_1 = \alpha/2mke >> 1, \quad u_2 = +1 \quad \text{and} \quad u_3 = -1.$$

Equation (3.8) with these substitutions becomes

$$\mathrm{Sn}^{-1}\left\{\left(\frac{u_o + 1}{2}\right)^{1/2} \Big/ \left(\frac{2}{\frac{\alpha}{2mke} + 1}\right)\right\} - \mathrm{Sn}^{-1}\left\{\left(\frac{u_\tau + 1}{2}\right)^{1/2} \Big/ \left(\frac{2}{\frac{\alpha}{2mke} + 1}\right)\right\} = c\ \mathrm{Tan}^{-1}\left\{\frac{2E}{\sqrt{\alpha}}\tau\right\} \tag{3.9}$$

where c is $\sqrt{\frac{mke}{2\alpha}\left(\frac{\alpha}{2mke} + 1\right)}$

As the parameter, $M = 2/(\frac{\alpha}{2meke} + 1)$, is very very small, when $\alpha/2mke >> 1$, we can approximate the above equation by substituting inverse sine functions, for inverse Sn elliptic functions. Also the constant c becomes equal to $1/2$, so (3.9) can be rewritten as

$$\mathrm{Sin}^{-1}\left\{\left(\frac{u_o + 1}{2}\right)^{1/2}\right\} - \mathrm{Sin}^{-1}\left\{\left(\frac{u_\tau + 1}{2}\right)^{1/2}\right\} = \pm \frac{1}{2}\,\mathrm{Tan}^{-1}\left(\frac{2E}{\sqrt{\alpha}}\tau\right) \tag{3.10}$$

Making the substitution $\tau = -\infty$, in (3.10) we get

$$\mathrm{Sin}^{-1}\left\{\left(\frac{u_o + 1}{2}\right)^{1/2}\right\} - \mathrm{Sin}^{-1}\left\{\left(\frac{u_{-\infty} + 1}{2}\right)^{1/2}\right\} = \mp \frac{\pi}{4} \tag{3.11}$$

We can use (3.11), to replace u_o in (3.10) and finally write $u(\tau)$. Thus

$$u_\tau = 2\,\mathrm{Sin}^2\left[\mathrm{Sin}^{-1}\left\{\left(\frac{u_{-\infty} + 1}{2}\right)^{1/2}\right\} \mp \frac{1}{2}\left\{\frac{\pi}{2} + \mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\,\tau\right\}\right] - 1 \tag{3.12}$$

We can also establish a relation between $u_{-\infty}$ and $u_{+\infty}$ which represent the cosines of the polar angles at times $\tau = -\infty$ and $+\infty$ respectively. Thus from (3.10), and (3.11), we have

$$\mathrm{Sin}^{-1}\left\{\left(\frac{u_{-\infty} + 1}{2}\right)^{1/2}\right\} - \mathrm{Sin}^{-1}\left\{\left(\frac{u_{+\infty} + 1}{2}\right)^{1/2}\right\} = \pm \frac{\pi}{2} \tag{3.13}$$

Application of (3.13) shows that deflection is zero for this case i.e., $\alpha/2mek >> 1$. This is what we should expect, for $\alpha/2mek >> 1$ corresponds to very large impact parameters. Since the dipole potential is weak, very large impact parameters will make the deflection practically zero. By making explicit calculations using (3.12), we can also show that the trajectory is nearly a straight line.

Case II $\alpha/2mke > 1$.

The roots arranged in descending order are $u_1 = \alpha/2mke$, $u_2 = 1$ and $u_3 = -1$.

Expressing u_o in terms of $u_{-\infty}$, (3.9) which covers the above case also can be written as

$$\mathrm{Sn}^{-1}\left\{\left(\frac{u_{-\infty}+1}{2}\right)^{1/2}\Big/M\right\} \mp c\left\{\frac{\pi}{2} + \mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\tau\right\}$$
$$= \mathrm{Sn}^{-1}\left\{\left(\frac{u_\tau+1}{2}\right)^{1/2}\Big/M\right\}; \quad M = 2/(\frac{\alpha}{2mke}+1). \tag{3.14}$$

So for $\alpha/2\,mek > 1$, we can write the trajectory as

$$r^2(\tau) = \frac{2E}{m}\tau^2 + \frac{\alpha}{2Em}$$

and

$$u(\tau) = 2\,\mathrm{Sn}^2\left[\mathrm{Sn}^{-1}\left\{\left(\frac{u_{-\infty}+1}{2}\right)^{1/2}\Big/M\right\} \mp c\left\{\frac{\pi}{2} + \mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\tau\right\}\right] - 1 \tag{3.15}$$

where

$$c = \sqrt{\frac{mke}{2\alpha}(u_1 - u_3)}.$$

(The negative sign with c when p_θ is initially positive, and the positive sign with c when p_θ is initially negative).

Case III. $\alpha/2mek = 1$.

This is a case of repeated roots with

$$u_1 = \alpha/2mek = u_2 = 1; \quad u_3 = -1.$$

and

$$f(u) = \left\{(u - 1)^2 (u + 1)\right\}^{1/2} .$$

The $(u - \tau)$ integral equation can be written as

$$\int_{u_o}^{u_\tau} \frac{du}{(u - 1)\sqrt{1 + u}} = -\sqrt{\frac{2mke}{\alpha}} \operatorname{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau \tag{3.16}$$

By changing the variable u to u', where $u' = u - 1$, the u integral in (3.16) can be reduced to a standard form and readily evaluated. Thus

$$\int_{u_o}^{u_\tau} \frac{du}{(u - 1)\sqrt{1 + u}} = \int_{u_{o-1}}^{u_{\tau-1}} \frac{du'}{u'\sqrt{u' + 2}}$$

and we finally get using (3.16)

$$\operatorname{Tanh}^{-1}\left\{\left(\frac{u_\tau + 1}{2}\right)^{1/2}\right\} = \operatorname{Tanh}^{-1}\left\{\left(\frac{u_{-\infty} + 1}{2}\right)^{1/2}\right\} \mp \frac{1}{\sqrt{2}}\left\{\frac{\pi}{2} + \operatorname{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau\right\} \tag{3.17}$$

So for this case of repeated roots, we have

$$r^2(\tau) = \frac{2E}{m} \tau^2 + \alpha/2Em,$$

and

$$u(\tau) = 2 \operatorname{Tanh}^2 \left[\operatorname{Tanh}^{-1}\left\{\left(\frac{u_{-\infty} + 1}{2}\right)^{1/2}\right\} \mp \frac{1}{\sqrt{2}}\left\{\frac{\pi}{2} + \operatorname{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau\right\}\right] - 1 \tag{3.18}$$

This "degeneration" of the inverse Sn functions to inverse Tan hyperbolic functions follows as a natural consequence of the relation $Sn(u/1) = Tanh(u)$, and the parameter $M = 2/(\frac{\alpha}{2mek} + 1)$ in the above case is 1. It should also be noted that (3.18) will not cover, the very special case, where motion is only along the axial line. For while $(\alpha/2mke) = 1$, in this case p_θ is always zero, and we recall from the $(\theta - \tau)$ integral equation, that p_θ should not be always zero, to evaluate the integral.

Case IV. $\alpha/2mek < 1$.

The roots arranged in descending order are

$u_1 = 1$, $u_2 = \frac{\alpha}{2mke}$ and $u_3 = -1$.

As before expressing u_o in terms of $u_{-\infty}$, (3.8) can be written as

$$Sn^{-1}\left\{\left(\frac{u_{-\infty} + 1}{\frac{\alpha}{2mek} + 1}\right)^{1/2} \Big/ M\right\} \mp c\left\{\frac{\pi}{2} + Tan^{-1}\frac{2E}{\sqrt{\alpha}}\tau\right\} = Sn^{-1}\left\{\left(\frac{u_\tau + 1}{\frac{\alpha}{2mek} + 1}\right)^{1/2} \Big/ M\right\} \quad (3.19)$$

where

$$c = \sqrt{\frac{mke}{\alpha}} \quad \text{and} \quad M = \left(\frac{\frac{\alpha}{2mek} + 1}{2}\right).$$

So for this case of $\alpha/2mek < 1$, we can write

$$u(\tau) = \left(\frac{\alpha}{2mek} + 1\right) Sn^2\left[\left\{Sn^{-1}\left(\frac{u_{-\infty} + 1}{\alpha/mek + 1}\right)^{1/2} \Big/ M\right\} \mp \sqrt{\frac{mke}{\alpha}}\left\{\frac{\pi}{2} + Tan^{-1}\frac{2E}{\sqrt{\alpha}}\tau\right\}\right] - 1$$

(3.20)

We have to note that, in this case, there is an upper bound for u value given by $\alpha/2mke$ and also $u_{-\infty}$ has to be $\leq \alpha/2mke$. Apart from the fact that an angular turning point given by $\theta = \cos^{-1}(\alpha/2mke)$ exists, the possibility of angular turnings (occuring 1 or more times before u_τ is reached) also exists. The number of times such angular turnings occur will depend upon how small $\alpha/2mek$ is, and also when $u(\tau)$ is calculated. Irrespective of the occurence of such angular turning points, $u(\tau)$ can be correctly evaluated using (3.20).

A study of the expressions for $r(\tau)$ and $u(\tau)$ indicates that for a given ion and given dipole strength, the trajectory can be traced, provided three parameters are fully specified. These are the energy E, the impact parameter $\underline{b}$ and the asymptotic angle $\theta_{-\infty}$. (If $b_{-\infty}$ is known in magnitude and direction, the sign of p_θ (initial) can be fixed). Before we close this section, we can make a passing reference to the case of $\sqrt{\alpha}$ being negative. Since the solution for the time integral is $(1/\sqrt{\alpha})\,\mathrm{Tan}^{-1}\{(2E/\sqrt{\alpha})\tau\}$, we find that the trajectory remains unaffected, whether $\sqrt{\alpha}$ is positive or negative.

C. The Orbit Equation

We can also write the orbit equation for motion in the meridian plane. We know from (2.12) that

$$p_\theta = \left(\frac{d\theta}{dr}\right) r \,(2Emr^2 - \alpha)^{1/2}$$

So the $(r - \theta)$ integral equation can be written as

$$\int_{r_{min}}^{r} \frac{dr}{r(2Emr^2 - \alpha)^{1/2}} = \int_{\theta_o}^{\theta} \frac{d\theta}{p_\theta} \quad . \tag{3.21}$$

The r integral can be evaluated easily by changing the variable r to γ, where $\cosh^2 \gamma = 2Emr^2/\alpha$. Then we get

$$\int_{r_{min}}^{r} \frac{dr}{r(2Emr^2 - \alpha)^{1/2}} = \frac{1}{\sqrt{\alpha}} \tan^{-1} \left\{ \left(\frac{2mE}{\alpha} r^2 - 1 \right)^{1/2} \right\}. \tag{3.22}$$

Using (3.6) we finally write the orbital equation as

$$c \tan^{-1}\left\{ \left(\frac{2mE}{\alpha} r^2 - 1 \right)^{1/2} \right\} = \pm \left[Sn^{-1}\left\{ \left(\frac{u_o - u_3}{u_2 - u_3} \right)^{1/2} \Big/ M \right\} - Sn^{-1}\left\{ \left(\frac{u - u_3}{u_2 - u_3} \right)^{1/2} \Big/ M \right\} \right] \tag{3.23}$$

where

$$c = \sqrt{\frac{mke\ (u_1 - u_3)}{2\alpha}}$$

and

$$M = \left(\frac{u_2 - u_3}{u_1 - u_3} \right).$$

Equation (3.23) can be written in a slightly different form as

$$r = r_{min} \operatorname{Sec} \left[\frac{1}{c}\, \delta - \frac{1}{c} Sn^{-1} \left\{ \left(\frac{u - u_3}{u_2 - u_3} \right)^{1/2} \Big/ M \right\} \right] \tag{3.24}$$

where δ is $Sn^{-1}\left\{\left(\frac{u_o - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\}$.

D. Special Orbit Equations

Here we will treat interesting coincidences of the radial turning point with either the axial line or the angular turning point.

Case A: If radial turning point occurs on the positive side of the axial line, i.e., on the line $\theta = o$, then we can write from (3.8),

$$K(M) - Sn^{-1}\left\{\left(\frac{u_\tau - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\} = c\ (Tan^{-1} \frac{2E}{\sqrt{\alpha}} \tau);\ u_o = u_2 = 1 \quad (3.25)$$

where $K(M)$ is $Sn^{-1}\ \{1/M\}$, and c is $\sqrt{\frac{u_1 - u_3)\ mke}{2\alpha}}$.

We know that

$$Tan^{-1}\left\{\frac{2E}{\alpha}\ (-\tau)\right\} = -Tan^{-1}\ (\frac{2E}{\sqrt{\alpha}}\ \tau) \quad .$$

So we can write from (3.25),

$$u_\tau = (u_2 - u_3)\ Sn^2\ \{K(M) - c\ Tan^{-1}\ (\frac{2E}{\sqrt{\alpha}}\ \tau)\}$$

and (3.26)

$$u_{-\tau} = (u_2 - u_3)\ Sn^2\ \{K(M) + c\ Tan^{-1}\ (\frac{2E}{\sqrt{\alpha}}\ \tau)\}$$

Since

$$Sn\ \{K(M) - c\ Tan^{-1}\ (\frac{2E}{\sqrt{\alpha}}\ \tau)\} = Sn\ \{\ K(M) + c\ Tan^{-1}\ (\frac{2E}{\sqrt{\alpha}}\ \tau)\}$$

We finally get

$$u_\tau = u_{-\tau} \quad . \tag{3.27}$$

Similarly when the radial turning point occurs on the negative side of the axial line, we can write from (3.8),

$$\mathrm{Sn}^{-1}\left\{\left(\frac{u_\tau - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\} = c\ \mathrm{Tan}^{-1}\left(\frac{2E}{\sqrt{\alpha}}\tau\right);\ u_o = u_3 = -1 \tag{3.28}$$

and from (3.28) it readily follows that

$$u_\tau = u_{-\tau} \quad .$$

So we can conclude, that when the radial turning point lies on the axial line, the orbit can be reflected about the axial vector. Figure 4a illustrates these orbits. We can also write the orbit equations from (3.24) as

$$r = r_{min}\ \mathrm{Sec}\left[\frac{K(M)}{c} - \frac{1}{c}\ \mathrm{Sn}^{-1}\left\{\left(\frac{u - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\}\right]\ ;\ u_o = u_2 = 1. \tag{3.29}$$

and

$$r = r_{min}\ \mathrm{Sec}\left[\frac{1}{c}\ \mathrm{Sn}^{-1}\left\{\left(\frac{u - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\}\right]\ ;\ u_o = u_3 = -1\ . \tag{3.30}$$

<u>Case B</u>: If the radial turning point coincides with the angular turning point, then we have $u_o = u_2 = \alpha/2mek$. We can find $u_{-\infty}$, from the $(u - \tau)$ integral equation. Thus we can write;

$$\int_{u_2 = u_o = \alpha/2mek}^{u_{-\infty}} - \frac{du}{\sqrt{f(u)}} = \sqrt{\frac{2mek}{\alpha}}\,\frac{\pi}{2};\ p_\theta \text{ is initially positive.} \quad (3.31)$$

We note that in the above equation u_o is the initial value of u at time $\tau = o$. But we can write

$$\int_{u_2}^{u_{-\infty}} - \frac{du}{\sqrt{f(u)}} \equiv \int_{u_3}^{u_2} \frac{du}{\sqrt{f(u)}} - \int_{u_3}^{u_{-\infty}} \frac{du}{\sqrt{f(u)}}$$

and so we finally write

$$K(M) - Sn^{-1}\left\{\left(\frac{u_{-\infty} - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\} = c\,\frac{\pi}{2}\ ;\ c = \sqrt{\frac{mke}{\alpha}}\ . \quad (3.32)$$

Whence

$$u_{-\infty} = (u_2 - u_3)\ Sn^2\left\{\left(K(M) - c\,\frac{\pi}{2}\right)\Big/ M\right\} + u_3\ . \quad (3.33)$$

From equation (3.8), we can write u_τ in terms of $u_{-\infty}$, and here $u_{-\infty}$ will be the initial value of u.

$$u_\tau = (u_2 - u_3)\ Sn^2\left[Sn^{-1}\left\{\left(\frac{u_{-\infty} - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\} \mp c\left\{\frac{\pi}{2} + Tan^{-1}\,\frac{2E}{\sqrt{\alpha}}\,\tau\right\}\right] + u_3\ .$$

(3.34)

If we substitute the value given for $u_{-\infty}$ in (3.33), in equation (3.34), we get

$$u_\tau = (u_2 - u_3)\ Sn^2\left[\left\{K(M) - c\,\frac{\pi}{2}\right\} \mp c\left\{\frac{\pi}{2} + Tan^{-1}\,\frac{2E}{\sqrt{\alpha}}\,\tau\right\}\right] + u_3 \quad (3.35)$$

Only if p_θ is initially negative, i.e., p_θ at time $\tau = -\infty$, we get

$$u_\tau = u_{-\tau} .$$

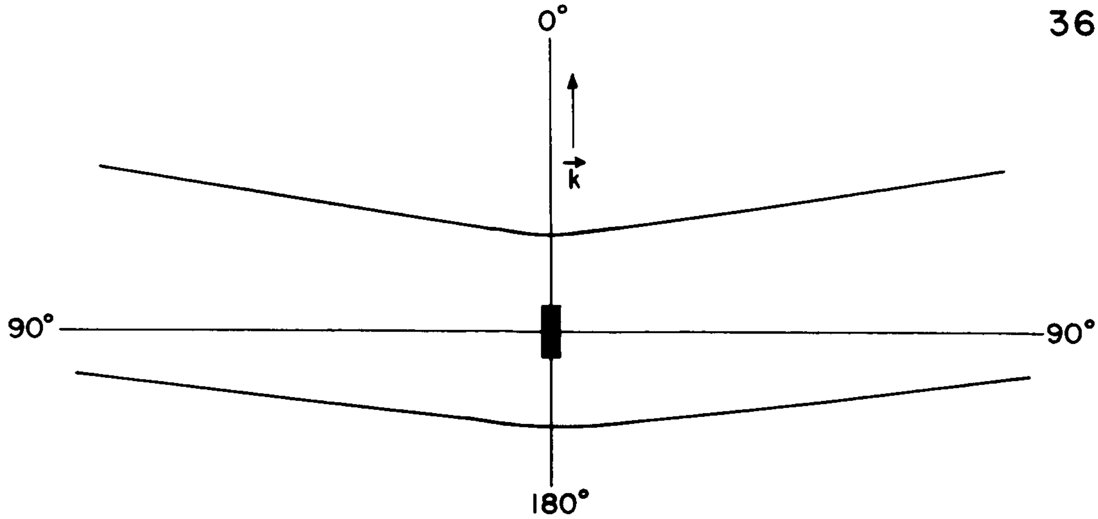
Also we know that $r_\tau = r_{-\tau}$. The only way in which these conditions can be satisfied is that when the ion reaches the common turning point, it should <u>retrace its path</u>. From (3.24), we can write the orbit equation for the above case as

$$r = r_{min} \operatorname{Sec}\left[\frac{1}{c} K(m) - \frac{1}{c} \operatorname{Sn}^{-1}\left\{\left(\frac{u - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\}\right] \tag{3.36}$$

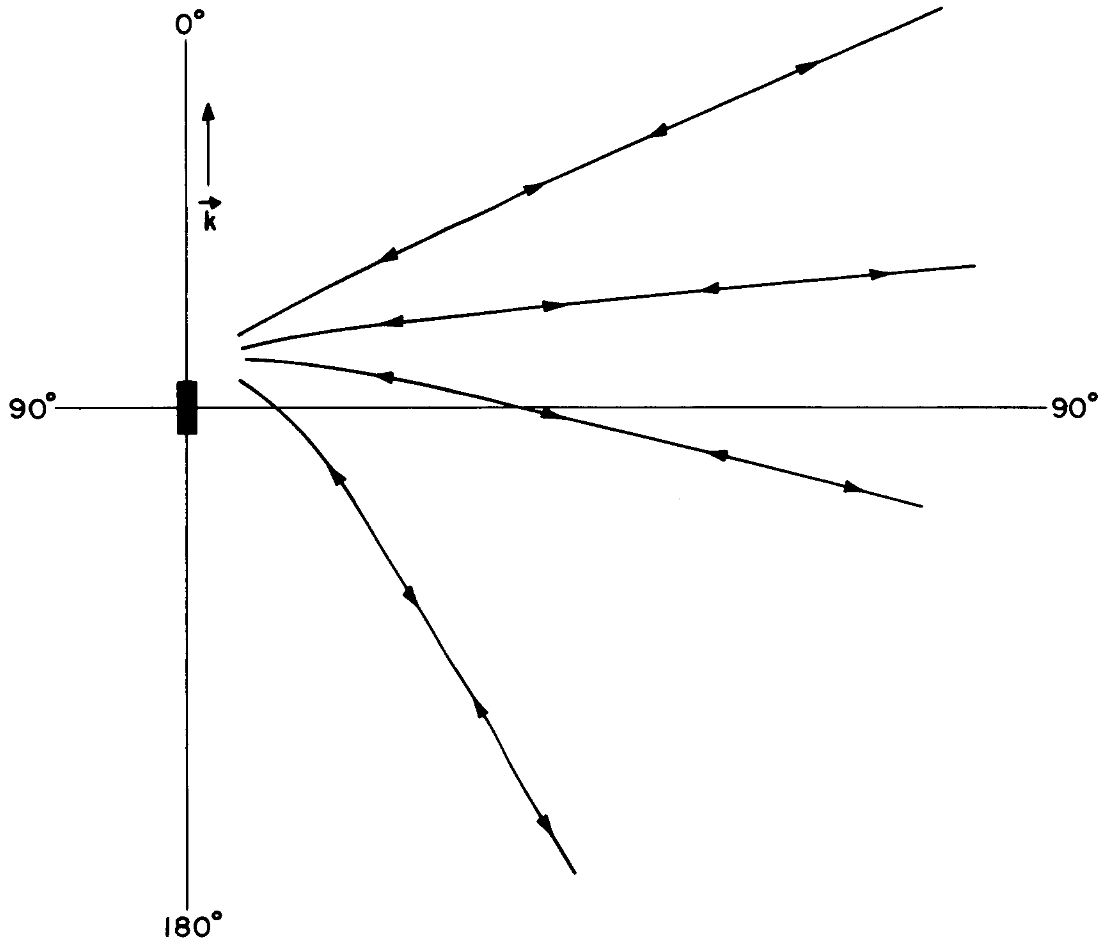
where

$$c = \sqrt{\frac{mke}{\alpha}} .$$

Figure 4b illustrates these orbits. These retracing orbits are curved because of the non-central nature of the dipole field; for central field problems, one is familiar only with <u>straight-line</u> retracing orbits (zero impact parameter) for the scattering problem.



(a). Reflection Of Certain Meridian Plane Oribits By Dipole Axis.



(b). Meridian Plane Orbits Retracing Their Curved Path After Reaching Their Common Turning Points. (i.e. $\dot{r}=0, \dot{\theta}=0$).

Figure 4. SPECIAL MERIDIAN PLANE ORBITS.

CHAPTER IV

NON-PLANAR MOTION

In this Chapter we deal with the motion of the ion when $p_\phi \neq o$. This means that, in general, the trajectory will not lie in a plane. To express θ as a function of time, we have to evaluate both sides of the integral

$$\int_{u_o}^{u_{\pm\infty}} \frac{\mp\, du}{(2mke)^{1/2}\left\{u^3 - \frac{\alpha}{2mke}u^2 - u + \frac{\alpha}{2mke} - \frac{p_\phi^2}{2mke}\right\}^{1/2}} = \int_{\tau=o}^{\tau=\pm\infty} \frac{d\tau}{2E\left(\tau^2 + \frac{\alpha}{4E^2}\right)} \quad . \tag{4.1}$$

For this we have to factor the cubic polynomial

$$f(u) = \{u^3 - \frac{\alpha}{2mke}u^2 - u + \frac{\alpha}{2mke} - \frac{p_\phi^2}{2mke}\} \quad .$$

We adopt the method given by Birkhoff and MacLane.[24] Let u_1, u_2 and u_3 be the roots of $f(u)$. Then

$$f(u) = \{(u - u_1)(u - u_2)(u - u_3)\} \equiv \{u^3 - \frac{\alpha}{2mke}u^2 - u + \frac{\alpha}{2mke} - \frac{p_\phi^2}{2mke}\} \quad . \tag{4.2}$$

Equating coefficients of like powers of u on both sides of the equation (4.2), we get

$$u_1 + u_2 + u_3 = \frac{\alpha}{2mke} \; ; \tag{4.3}$$

$$u_1 u_2 + u_2 u_3 + u_3 u_1 = -1 \tag{4.4}$$

$$u_1 u_2 u_3 = \frac{p_\phi^2 - \alpha}{2mke} \quad . \tag{4.5}$$

From (4.3), we have

$$u_2 + u_3 = \frac{\alpha}{2mke} - u_1 \quad . \tag{4.6}$$

Also from (4.5),

$$u_2 u_3 = \left(\frac{p_\phi^2 - \alpha}{2mke} \right) \frac{1}{u_1} \quad . \tag{4.7}$$

Therefore

$$(u_2 - u_3) = \pm \left\{ \left(\frac{\alpha}{2mke} - u_1 \right)^2 - \frac{4}{u_1} \left(\frac{p_\phi^2 - \alpha}{2mke} \right) \right\}^{1/2}$$

or

$$(u_2 - u_3) = \pm \left\{ \frac{\alpha^2}{4m^2k^2e^2} + \frac{2\alpha}{mke}\frac{1}{u_1} - \frac{\alpha}{mke} u_1 + u_1^2 - \frac{2p_\phi^2}{mke}\frac{1}{u_1} \right\}^{1/2} \quad . \tag{4.8}$$

Solving the two simultaneous equations in u_2 and u_3 given by (4.6) and (4.8) we write,

$$u_2 = \frac{1}{2}\left(\frac{\alpha}{2mke} - u_1\right) + \frac{1}{2}\left\{\frac{\alpha^2}{4m^2k^2e^2} + \frac{2\alpha}{mke}\frac{1}{u_1} - \frac{\alpha u_1}{mke} + u_1^2 - \frac{2p_\phi^2}{mke}\frac{1}{u_1}\right\}^{1/2} \qquad (4.9)$$

and

$$U_3 = \frac{1}{2}\left(\frac{\alpha}{2mke} - u_1\right) - \frac{1}{2}\left\{\frac{\alpha^2}{4m^2k^2e^2} + \frac{2\alpha}{mke}\frac{1}{u_1} - \frac{\alpha u_1}{mke} + u_1^2 - \frac{2p_\phi^2}{mke}\frac{1}{u_1}\right\}^{1/2} \qquad (4.10)$$

We can write it in the above way, because if the negative root in (4.8) is taken, only u_2 and u_3 will get interchanged and this is immaterial.

To complete the factorization we have to determine u_1. Since u_1 is one of the roots of the cubic polynomial $f(u)$, we can write

$$2\ mke\ u_1^3 - \alpha u_1^2 - 2\ mke\ u_1 + \alpha - p_\phi^2 = 0 \qquad (4.11)$$

The square term in (4.11) can be eliminated by making the substitution,

$$u_1 = d + \frac{\alpha}{2mke}\ \frac{1}{3}\ . \qquad (4.12)$$

With the above substitution, and rearrangement of terms (4.11) reduces to

$$d^3 - d\left(\frac{\alpha^2}{12m^2k^2e^2} + 1\right) = \frac{\alpha^3}{108m^3k^3e^3} - \frac{\alpha}{3mke} + \frac{p_\phi^2}{2mke}\ . \qquad (4.13)$$

Equation (4.13) can be transformed still further to obtain simple trigonometric or hyperbolic solutions. To effect this transformation, we substitute

$$he' = d \ ; \quad h = \left(\frac{4}{3}\right)^{1/2} \left(\frac{\alpha^2}{12m^2k^2e^2} + 1\right)^{1/2} \tag{4.14}$$

in (4.13) and then multiply both sides of the resulting equation by

$$n = \frac{3\sqrt{3}}{2} \frac{1}{\left(\frac{\alpha^2}{12m^2k^2e^2} + 1\right)} \ . \tag{4.15}$$

With these operations (4.13) reduces to

$$4e'^2 - 3e' = f; \quad f = \left(\frac{\alpha^3}{108m^3k^3e^3} - \frac{\alpha}{3mke} + \frac{p_\phi^2}{2mke}\right) \frac{\sqrt{27}}{2} \frac{1}{\left(\frac{\alpha^2}{12m^2k^2e^2} + 1\right)^{3/2}} \tag{4.16}$$

The solution for e' will depend upon the value of the constant f given in (4.16).

Thus if f is $\geqslant 1$,

$$e' = \cosh\left[\left(\frac{1}{3}\right) \cosh^{-1} f\right] \tag{4.17}$$

If $|f|$ is less than 1, the solution is

$$e' = \cos\left[\left(\tfrac{1}{3}\right)\cos^{-1} f\right] \quad . \tag{4.18}$$

If $f \leqslant -1$, then the solution is

$$-e' = \cosh\left[\left(\tfrac{1}{3}\right)\cosh^{-1} f\right] \tag{4.19}$$

From (4.12) and (4.14), we get

$$u_1 = e'\left[\left(\frac{4}{3}\right)\left\{\frac{\alpha^2}{12m^2k^2e^2} + 1\right\}\right]^{1/2} + \frac{\alpha}{6\ mke} \quad . \tag{4.20}$$

Of the possible solutions for e, (4.19) where f is $\leqslant -1$ can be ruled out for our problem. (This can be shown by studying the form of f given in (4.16) and also noting that α has to be always positive.)

Making the substitution for e' given in (4.17) and (4.18), the complete solution for u_1 can be written as

$$u_1 = \frac{\alpha}{6mke} + \left\{\frac{4}{3}\left(\frac{\alpha^2}{12m^2k^2e^2} + 1\right)\right\}^{1/2} \begin{matrix}\cosh \\ \text{or} \\ \cos\end{matrix} \left[\left(\frac{1}{3}\right) \begin{matrix}\cosh^{-1} \\ \text{or} \\ \cos^{-1}\end{matrix} (f)\right] \quad . \tag{4.21}$$

according as $f \geqslant 1$ or $|f|$ is < 1.

The other roots u_2 and u_3 follow from (4.9) and (4.10).

$$u_2 = \frac{\alpha}{4mke} - \frac{u_1}{2} + \frac{1}{2}\left\{\frac{\alpha^2}{4m^2k^2e^2} + \frac{2\alpha}{mke\ u_1} - \frac{\alpha u_1}{mke} + u_1^2 - \frac{2p_\phi^2}{mke\ u_1}\right\}^{1/2}$$

$$u_3 = \frac{\alpha}{4mke} - \frac{u_1}{2} - \frac{1}{2}\left\{\frac{\alpha^2}{4m^2k^2e^2} + \frac{2\alpha}{mke\ u_1} - \frac{\alpha u_1}{mke} + u_1^2 - \frac{2p_\phi^2}{mke\ u_1}\right\}^{1/2}$$

As a check, we can also show that

$$\text{as} \quad p_\phi \to o, \qquad u_1 \to \frac{\alpha}{2mke},$$

$$u_2 \to 1 \quad \text{and}$$

$$u_3 \to -1;$$

i.e., we obtain the very same roots that we got previously when we considered motion in the meridian plane.

A. Effect of p_ϕ on the Roots of the Cubic Polynomial

From (4.16) it is evident that for the case $p_\phi \neq o$, the value of f will be more than for the case $p_\phi = o$. It follows easily from (4.21) that u_1 will be greater than $\alpha/2mek$, which is the value it will take when $p_\phi = o$. Again regarding the roots for the case $p_\phi \neq o$, it is evident from 4.22, that u_2 should decrease below the value it will take when $p_\phi = o$, and u_3 will increase above the value it will take when $p_\phi = o$. So

$$u_2 < 1; \quad u_3 > -1 .$$

The cubic polynomial $f(u)$ will look like Figure 5a or 5b or 5c, according as p_ϕ^2 is less than α, or equal to α or greater than α. For motion to take place $f(u)$ must be positive, and one can see from Figure 5, that u has to lie between u_2 and u_3. It is evident from these figures that the effect of p_ϕ being non zero is

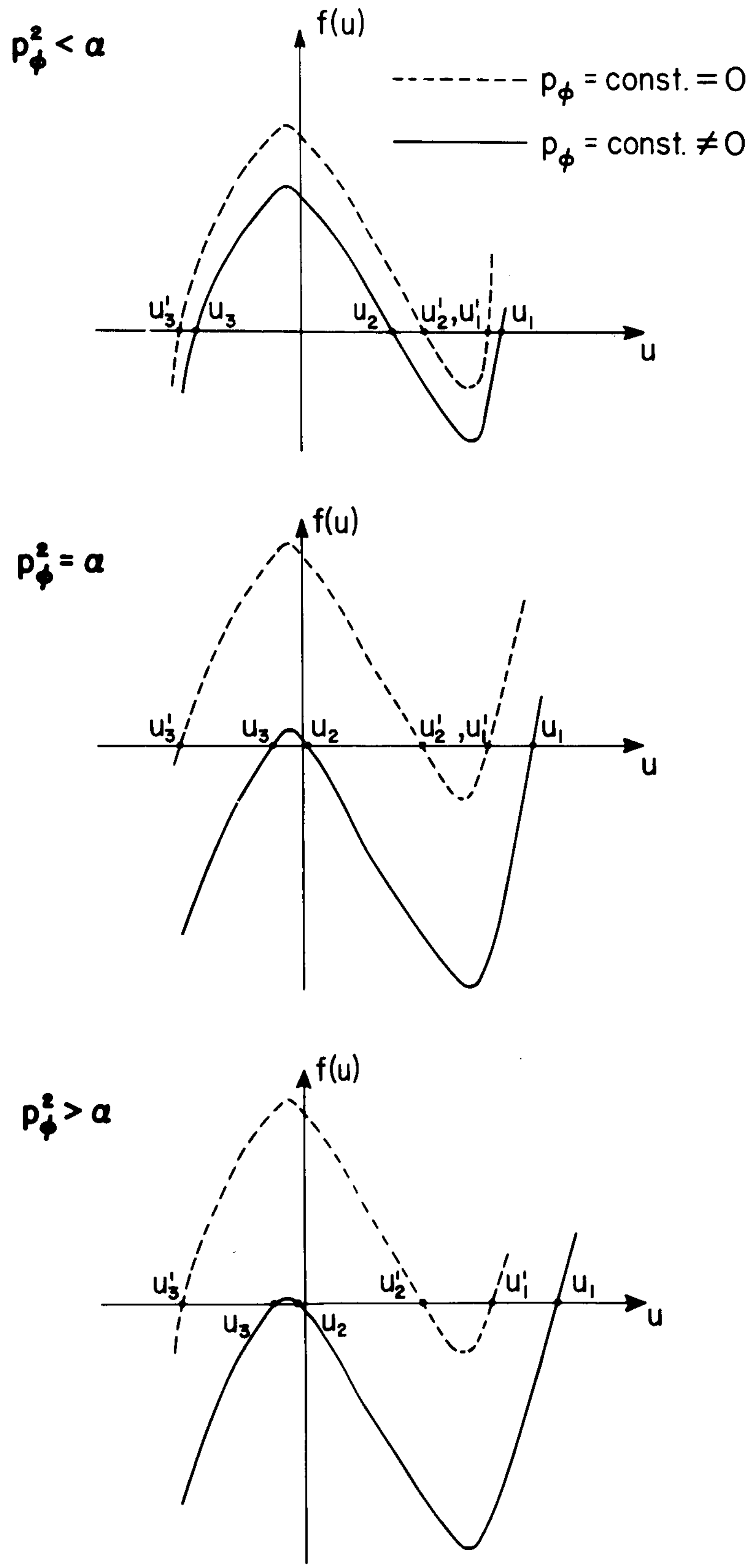


Figure 5. f(u) For Non-Planar Motion.

to restrict the range of value for θ. Thus

$$\theta_1 \leqslant \theta \leqslant \theta_2 \;; \quad (\theta_1 = \cos^{-1}(u_2) \text{ and it is more than } 0°.$$
$$\theta_2 = \cos^{-1}(u_3) \text{ and it is less than } 180°).$$

B. Determination of p_ϕ

The roots u_1, u_2 and u_3 can be determined provided p_ϕ is known. p_ϕ or the z component of the total angular momentum is given by

$$p_\phi = \hat{\varepsilon}_3 \cdot (\vec{r} \times m\vec{v}),$$

where $\hat{\varepsilon}_3$ is unit vector in the direction of the dipole axis. We can determine p_ϕ from the initial conditions of the problem. Thus if $\vec{b}$ be the initial impact parameter and $\vec{V}$, the initial velocity at time $\tau = -\infty$, then

$$p_\phi = \varepsilon_3 \cdot (\vec{b} \times m\vec{v}). \tag{4.22}$$

The components of $\vec{v}$ at time $\tau = -\infty$ will be

$$\vec{v} = \sqrt{\left(\frac{2E}{m}\right)} \sin \theta_{-\infty} \cos \phi_{-\infty} \hat{\varepsilon}_1, \sqrt{\left(\frac{2E}{m}\right)} \sin \theta_{-\infty} \sin \phi_{-\infty} \hat{\varepsilon}_2 \text{ and } \sqrt{\left(\frac{2E}{m}\right)} \cos \theta_{-\infty} \hat{\varepsilon}_3 \tag{4.23}$$

where ε_1, ε_2, and ε_3 are unit vectors along the coordinate axes x, y and z respectively, $\theta_{-\infty}$ and $\phi_{-\infty}$ are the polar and the azimuthal angles indicating the position of the ion at time $\tau = -\infty$. So p_ϕ can be determined if $\vec{b}$, the impact parameter is fully specified in addition to specifying $\theta_{-\infty}$ and $\phi_{-\infty}$.

With the roots completely evaluated, θ can be expressed as a function of time τ.

$$u_\tau = (u_2 - u_3)\ \mathrm{Sn}^2\left[\mathrm{Sn}^{-1}\left\{\left(\frac{u_{-\infty} - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\} \mp c\left\{\frac{\pi}{2} + \mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\tau\right\}\right] + u_3\ . \tag{4.24}$$

where

$$c = \sqrt{\frac{mke\ (u_1 - u_3)}{2\alpha}}$$

and

$$M = \frac{u_2 - u_3}{u_1 - u_3}\ ,$$

and

$$u_1 > u_2 > u_3 .$$

(The negative sign with c is for the case p_θ positive initially and the positive sign for the case p_θ negative initially. Here after for convenience we will consider only p_θ positive case.)

C. ϕ as a Function of Time

We have already seen that p_ϕ is conserved, and from the Hamiltonian (1.1),

$$\frac{\partial H}{\partial p_\phi} = \dot{\phi} = \frac{p_\phi}{mr^2 \sin^2\theta} .$$

Therefore,

$$p_\phi = mr^2 \sin^2\theta \, \dot{\phi} . \tag{4.25}$$

So the $(\phi - \tau)$ integral equation becomes

$$\int_{\phi-\infty}^{\phi(\tau)} \frac{d\phi}{p_\phi} = \int_{\tau=-\infty}^{\tau} \frac{d\tau}{mr^2(\tau) \sin^2\theta(\tau)} \tag{4.26}$$

$\sin^2 \theta(\tau)$ required in (4.26) can be expressed in a simple form, by making suitable substitutions.

Thus we note that,

$$\sin^2\theta(\tau) = (1 - u_\tau)(1 + u_\tau) . \tag{4.27}$$

Let

$$Sn^{-1}\left\{\left(\frac{u_{-\infty} - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\} - c\,\frac{\pi}{2} \text{ be } = \gamma \tag{4.28}$$

and

$$\text{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau = \tau' \quad . \tag{4.29}$$

With the substitutions given in (4.28) and (4.29), and using (4.24), (4.27) can be rewritten as

$$\sin^2\theta(\tau) = \{(1+u_3) + (u_2-u_3)\,\text{Sn}^2\,(\gamma-c\tau')\} \times \{(1-u_3) - (u_2-u_3)\,\text{Sn}^2\,(\gamma-c\tau')\} \quad . \tag{4.30}$$

The variable τ can be changed to τ' defined in (4.29) and the integral equation (4.26) reduces to

$$\phi(\tau) = \phi_{-\infty} + \frac{p_\phi}{\sqrt{\alpha}} \int_{-\frac{\pi}{2}}^{\text{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau} \frac{d\tau'}{\{(1+u_3) + (u_2-u_3)\text{Sn}^2(\gamma-c\tau')\}\{(1-u_3) - (u_2-u_3)\text{Sn}^2(\gamma-c\tau')\}} \; . \tag{4.31}$$

The integration variable τ' can be once more changed to τ'' where

$$\gamma - c\tau' = \tau'', \tag{4.32}$$

and (4.31) can be rewritten as

$$\phi(\tau) = \phi_{-\infty}$$

$$- \frac{p_\phi}{c\sqrt{\alpha}} \frac{1}{(1-u_3^2)} \int_{\gamma + \frac{c\pi}{2}}^{\gamma - c \,\mathrm{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau} \frac{d\tau''}{\left\{1 - \left(\frac{u_2-u_3}{1-u_3}\right) \mathrm{Sn}^2\tau''\right\} \left\{1 + \left(\frac{u_2-u_3}{1+u_3}\right) \mathrm{Sn}^2\tau''\right\}} \; . \tag{4.33}$$

Let

$$\frac{u_2-u_3}{1-u_3} = a; \quad \frac{u_2-u_3}{1+u_3} = b \tag{4.34}$$

Then

$$\phi(\tau) = \phi_{-\infty}$$

$$- \frac{p_\phi}{c\sqrt{\alpha}} \frac{1}{(1-u_3^2)} \frac{1}{(a+b)} \int_{\gamma + \frac{c\pi}{2}}^{\gamma - c \,\mathrm{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau} d\tau'' \left\{ \frac{a}{(1-a\mathrm{Sn}^2\tau'')} + \frac{b}{(1+b\mathrm{Sn}^2\tau'')} \right\} . \tag{4.35}$$

With the substitutions for a and b given in (4.34), (4.35) can be re-written as

$$\phi(\tau) = \phi_{-\infty} - \frac{p_\phi}{c\sqrt{\alpha}} \frac{1}{2(1-u_3)} \int_{\gamma+\frac{c\pi}{2}}^{\gamma - c\,\mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\tau} \frac{d\tau''}{1-a\mathrm{Sn}^2\tau''}$$

$$- \frac{p_\phi}{c\sqrt{\alpha}} \frac{1}{2(1+u_3)} \int_{\gamma+\frac{c\pi}{2}}^{\gamma - c\,\mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\tau} \frac{d\tau''}{1+b\mathrm{Sn}^2\tau''} \tag{4.36}$$

This is equivalent to writing

$$\phi(\tau) = \phi_{-\infty} + \frac{p_\phi}{c\sqrt{\alpha}}\left[\left\{\frac{1}{2(1-u_3)} \int_0^{\gamma+\frac{c\pi}{2}} \frac{d\tau''}{1-a\mathrm{Sn}^2\tau''}\right\} + \left\{\frac{1}{2(1+u_3)} \int_0^{\gamma+\frac{c\pi}{2}} \frac{d\tau''}{1+b\mathrm{Sn}^2\tau'}\right\}\right]$$

$$- \frac{p_\phi}{c\sqrt{\alpha}}\left[\left\{\frac{1}{2(1-u_3)} \int_0^{\gamma - c\,\mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\tau} \frac{d\tau''}{1-a\mathrm{Sn}^2\tau''}\right\} + \left\{\frac{1}{2(1+u_3)} \int_0^{\gamma - c\,\mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\tau} \frac{d\tau''}{1+b\mathrm{Sn}^2\tau''}\right\}\right] \tag{4.37}$$

The above integrals are of the form

$$\int_0^{u_1} \frac{du}{1-\beta^2\mathrm{Sn}^2 u},$$

where β^2 can take positive or negative value. These are known as incomplete elliptic integrals of the third kind in Legendre's canonical form, and the solution is

$$\int_0^{u_1} \frac{du}{1-\beta^2 Sn^2 u} = \Pi\,(u_1,\beta^2) \quad \text{for} \quad [-\infty < \beta^2 < \infty]. \tag{4.38}$$

The exact form which the function $\Pi(u_1,\beta^2)$ will take will depend upon which one of the six cases given underneath is valid.

$$\left.\begin{array}{ll} \text{Case i} & 0 < -\beta^2 < \kappa \\ \text{Case ii} & \kappa < -\beta^2 < \infty \\ \text{Case iii} & 0 < \kappa < \beta^2 < 1 \\ \text{Case iv} & 0 < \kappa^2 < \beta^2 < \kappa \\ \text{Case v} & 0 < \beta^2 < \kappa^2 \\ \text{Case vi} & \infty > \beta^2 > 1 \end{array}\right\} \quad \text{Here} \quad \kappa^2(M) = \left(\frac{u_2-u_3}{u_1-u_3}\right).$$

So knowing the roots u_1, u_2 and u_3 of the cubic polynomial, (4.37) can be evaluated to give ϕ as a function of time τ. Thus

$$\phi(\tau) = \phi_{-\infty} + \frac{p_\phi}{(1-u_3)\{2(u_1-u_3)mke\}^{1/2}} \left[\frac{1}{(1-u_3)} \Pi(\gamma + \frac{c\Pi}{2}, \beta^2 = a) + \frac{1}{(1+u_3)} \Pi(\gamma + \frac{c\Pi}{2}, -\beta^2 = b) \right.$$

$$\frac{-p_\phi}{(1-u_3)\sqrt{2mke\,(u_1-u_3)}} \left[\frac{1}{(1-u_3)} \Pi(\gamma - c\, \mathrm{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau, \beta^2 = a) + \frac{1}{(1+u_3)} \Pi(\gamma - c\, \mathrm{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau, -\beta^2 = b) \right].$$

(4.39)

The $\Pi(u_1, \beta^2)$ functions for different cases are all given by Byrd and Friedman.[25]

CHAPTER V

GRAPHICAL REPRESENTATION OF ORBITS AND DEFLECTION ANGLES

In this Chapter we first discuss in sections A and B a few specific calculations of trajectories for motion in the meridian plane and then show in section C a special case of non-planar motion: $\alpha = p_\phi^2$ with $u_o = 0$.

A. Angular Dependence of Meridian Plane Orbits:

We know that the equation

$$u_\tau = (u_2 - u_3)\ Sn^2\left[Sn^{-1}\left\{\left(\frac{u_{-\infty} - u_3}{u_2 - u_3}\right)^{1/2} M\right\} \mp c\left\{\frac{\pi}{2} + Tan^{-1}\frac{2E}{\sqrt{\alpha}}\tau\right\}\right] + u_3$$

enables us to calculate u_τ, and consequently trace the trajectory, provided $u_{-\infty}$ and the initial sign of p_θ are known. The above equation illustrates that for a given impact parameter the trajectory is strongly angular dependent, in the sense that it depends upon the initial value $u_{-\infty}$. Table I gives the values of r and θ at different times for different choices of $\theta_{-\infty}$, for the case of motion in the meridian plane. (We have chosen an impact parameter of 0.5 Ångstrom and an ion energy of 100 electron volts. The dipole moment of water molecule has been taken to be 1.85×10^{-18} e. s. u. - c.m. units; p_θ is initially positive for all $\theta_{-\infty}$ except for 180^o) Figure 6 gives the meridian plane trajectories of the ion for these angles $\theta_{-\infty}$

equal to 0°, 45°, 90°, 135° and 180°. One can see from figure 6 that, at large distances from the force center, the orbits are nearly straight lines which is what one would expect. Also when the ion is near the force center, it curves inwards, if it happens to be in the attractive hemisphere, and curve outwards when it is in the repulsive hemisphere.

Table II gives the angles of deflection, $\Theta = 180^{\circ} - (\theta_{-\infty} - \theta_{+\infty})$, for different values of Eb^2. (P_{θ} is initially positive for every case except for $\theta_{-\infty}$ equal to 180°). A plot of deflection angle Θ versus Eb^2, for different asymptotic angles $\theta_{-\infty}$, is given in Figure 7. Both the figures 6 and 7 illustrate that, for a given Eb^2, the deflection angle Θ is maximum, when the ion is initially on the equatorial line, and minimum when it is on the positive side of the axial line, i.e., $\theta_{-\infty}$ is 0°. It is also seen that the deflection of the ion is greater when $\theta_{-\infty}$ is 135°, than when it is 45°. Similarly, Θ is greater for $\theta_{-\infty}$ equal to 180°, than for $\theta_{-\infty}$ equal to 0°. Figure 7 also shows how the angle of deflection falls with increase in Eb^2.

TABLE I

Orbit Data for Different Asymptotic Angles (Meridian Plane Orbits: $p_{\phi} = 0$)

Impact Parameter = 0.5A°, Ion Energy = 100 e.v., Dipole Moment = 1.85×10^{-18} e.s.u-cm.

Time in 10^{-16} secs	$\theta_{-\infty} = 0^{\circ}$		$\theta_{-\infty} = 45^{\circ}$		$\theta_{-\infty} = 90^{\circ}$		$\theta_{-\infty} = 135^{\circ}$		$\theta_{-\infty} = 180^{\circ}$	
	r in Au	θ	r in Au	θ	r in Au	θ	r in Au	θ	r in Au	θ
$-\infty$	∞	0°-00	∞	45°-00	∞	90°-00	∞	135°-00	∞	180°-00
-1000.00	138.42	1°-36'	138.42	45°-12'	138.42	90°-12'	138.42	135°-12'	138.42	179°-49'
- 100.00	13.85	2°-30'	13.85	47°-04'	13.85	92°-04'	13.85	137°-04'	13.85	177°-51'
- 75.00	10.40	3°-06'	10.40	47°-45'	10.39	92°-46'	10.39	137°-47'	10.39	177°-12'
- 50.00	6.94	4°-24'	6.94	49°-26'	6.94	94°-09'	6.94	139°-09'	6.94	177°-07'
- 25.00	3.50	8°-18'	3.50	53°-15'	3.50	98°-17'	3.49	143°-16'	3.49	171°-46'
- 10.00	1.49	19°-47'	1.48	65°-01'	1.47	110°-15'	1.46	155°-14'	1.45	160°-00'
- 7.50	1.18	25°-29'	1.17	70°-57'	1.15	116°-22'	1.14	161°-22'	1.13	153°-59'
- 5.00	.89	35°-12'	.88	81°-10'	.854	127°-04'	.83	172°-13'	.82	143°-24'
- 2.50	.65	53°-13'	.64	100°-35'	.608	148°-03'	.57	165°-55'	.56	122°-15'
- 1.00	.57	70°-26'	.56	119°-31'	.519	169°-11'	.48	143°-26'	.46	100°-30'

TABLE I CONTINUED

Time in 10^{-16} secs	$\theta_{-\infty} = 0°$		$\theta_{-\infty} = 45°$		$\theta_{-\infty} = 90°$		$\theta_{-\infty} = 135°$		$\theta_{-\infty} = 180°$	
	r in Au	θ	r in Au	θ	r in Au	θ	r in Au	θ	r in Au	θ
0	.55	84°-13'	.54	134°-46'	.500	173°-42'	.46	125°-11'	.44	83°-00'
1.00	.57	98°-19'	.56	150°-15'	.519	156°-41'	.48	107°-27'	.46	66°-16'
2.50	.65	116°-48'	.64	170°-10'	.608	135°-47'	.57	86°-54'	.56	47°-14'
5.00	.89	137°-09'	.88	168°-41'	.854	115°-06'	.83	68°-01'	.82	30°-11'
7.50	1.18	148°-30'	1.17	157°-18'	1.15	104°-35'	1.14	58°-55'	1.13	22°-04'
10.00	1.49	155°-14'	1.48	150°-38'	1.47	98°-36'	1.46	53°-50'	1.45	17°-32'
25.00	3.50	169°-00	3.50	137°-17'	3.50	86°-53'	3.49	44°-01'	3.49	9°-00'
50.00	6.94	173°-54'	6.94	132°-44'	6.94	82°-51'	6.94	40°-39'	6.94	6°-15'
75.00	10.40	175°-32'	10.40	131°-03'	10.39	81°-29'	10.39	39°-31'	10.39	5°-24'
100.00	13.85	176°-21'	13.85	130°-16'	13.85	80°-49'	13.85	38°-57'	13.85	5.00
1000.00	138.42	178°-37'	138.42	128°-08'	138.42	78°-59'	138.42	37°-26'	138.42	4.00
∞	∞	178°-51'	∞	127°-54'	∞	78°-47'	∞	37°-16'	∞	3°-54'

p_θ , initially positive for all values of $\theta_{-\infty}$ except 180°

Impact parameter b = .5Au for all cases

E = 100 electron volts

k = 1.85×10^{-18} esu-cm

m = 1.67×10^{-24} gms

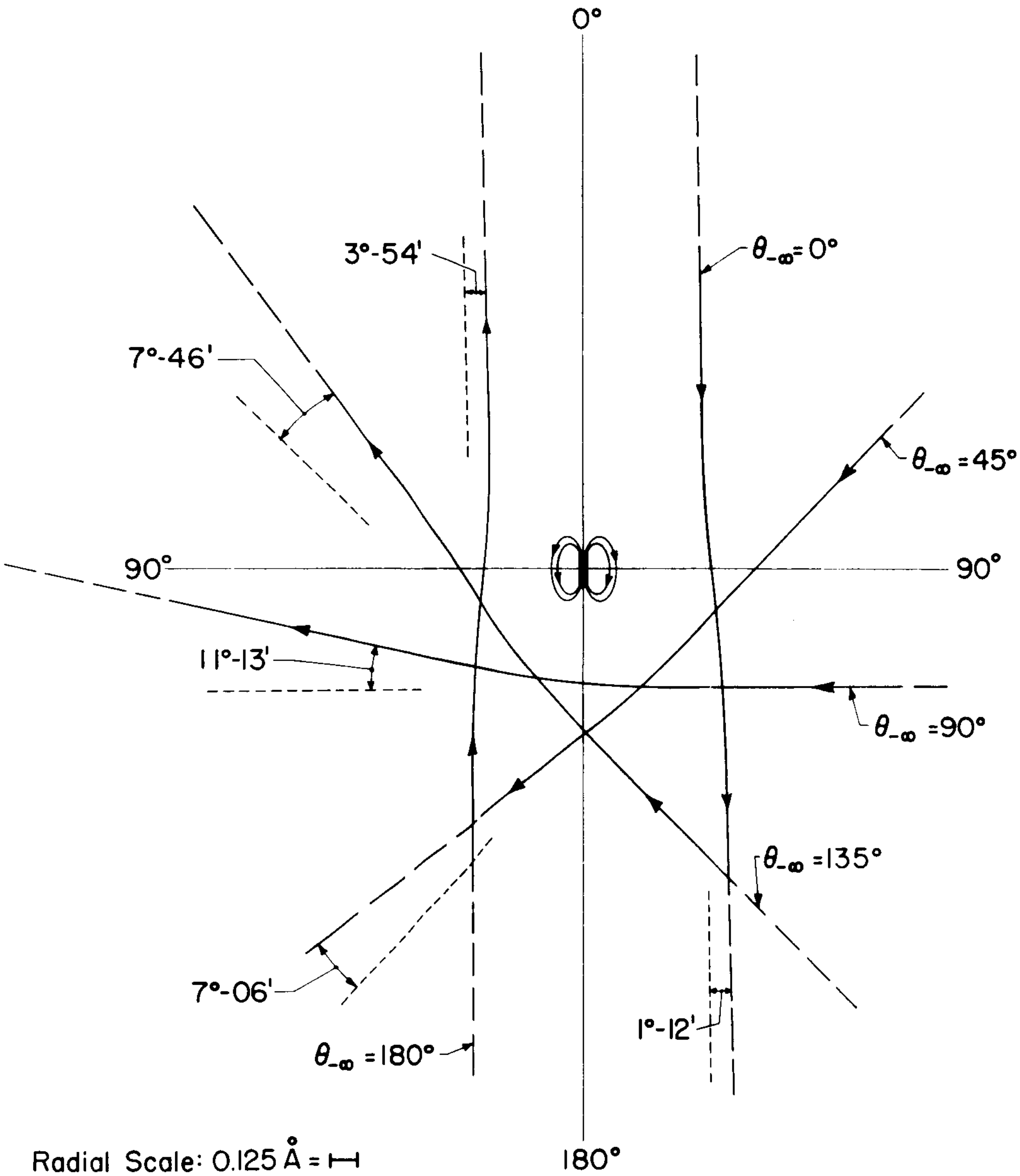


Figure 6. Meridian Plane Orbits For Different Values Of $\theta_{-\infty}$.

TABLE II

Variation of Deflection Angle Θ with Eb^2 and $\theta_{-\infty}$

Eb^2 ev-(Au^2) units	$\theta_{-\infty}=0^o$	$\theta_{-\infty}=45^o$	$\theta_{-\infty}=90^o$	$\theta_{-\infty}=135^o$	$\theta_{-\infty}=180^o$
	Θ_+	Θ_+	Θ_+	Θ_+	Θ_+
12.25	3^o-54'	11^o-43'	19^o-53'	12^o-15'	17^o-45
16.00	2^o-32'	9^o-52'	16^o-15'	10^o-24'	8^o-00
20.25	1^o-42'	8^o-20'	13^o-24'	9^o-06'	5^o-24'
25.00	1^o-12'	7^o-06'	11^o-13'	7^o-46'	3^o-54'
36.00	0^o-36'	5^o-18'	8^o-09'	5^o-45'	1^o-55'
49.00	0^o-18	4^o-06'	6^o-08'	4^o-22'	0^o-33'
64.00		3^o-14'	4^o-47'	3^o-24'	
100.00		2^o-10'	3^o-06'	2^o-15'	
144.00		1^o-32'	2^o-12'	1^o-35'	
196.00		1^o-09'	1^o-40'	1^o-11'	
256.00		0^o-54'	1^o-18'	0^o-55'	
324.00		0^o-44'	1^o-03'	0^o-44'	
400.00		0^o-37'	0^o-52'	0^o-36'	
900.00		0^o-19'	0^o-24'	0^o-19'	

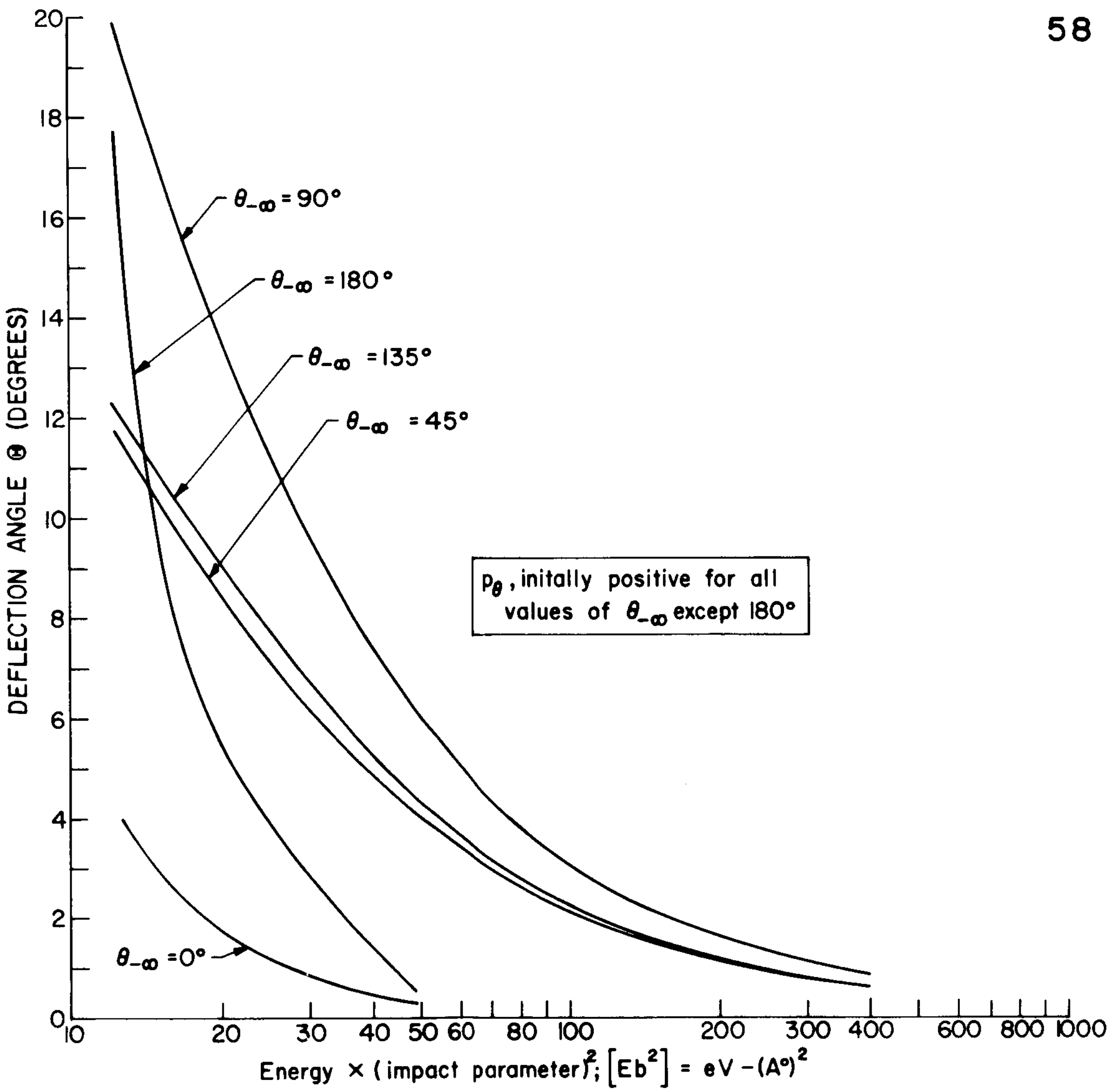


FIGURE 7. DEFLECTION ANGLE AS A FUNCTION OF Eb^2.

B. Dependence on the Sign of Initial p_θ for Meridian Plane Orbits

The expression for u_τ indicates clearly that the value of u_τ depends on the initial sign of p_θ. So for the same Eb^2 and $\theta_{-\infty}$, we will in general get two different trajectories, which correspond to p_θ being initially either positive or negative. It should be noted that this is not so when $\theta_{-\infty}$ happens to be either 0° or 180°. When $\theta_{-\infty}$ is 0°, then p_θ has to be initially positive, while for the case of $\theta_{-\infty}$ equal to 180°, p_θ has to be initially negative, and so for these cases there is only one orbit for a given Eb^2. (There is also the trivial case of motion along the axial line corresponding to p_θ being always zero.) Table III gives the (r-θ) orbit data, both for p_θ initially positive and negative. Figure 8 gives both the trajectories for each one of the asymptotic angles $\theta_{-\infty}$, namely 45°, 90° and 135°. The orbits for p_θ initially negative also demonstrate the tendency to curve inwards when the ion is near the force center, in the attractive hemisphere, and curve outwards when the ion is near the force center on the repulsive hemisphere.

TABLE III

Comparative Orbital Data for p_θ Initially Positive and Negative (Meridian Plane Orbits: $p_\phi = 0$)

Impact Parametor = 0.5A°, Ion Energy - 100 e.v., Dipole Moment = 1.85×10^{-18} e.s.u-cm.

Time in 10^{-16} secs	$\theta_{-\infty} = 45°$			$\theta_{-\infty} = 90°$			$\theta_{-\infty} = 135°$		
		p_θ positive	p_θ negative		p_θ positive	p_θ negative		p_θ positive	p_θ negative
	r in Au	θ	θ	r in Au	θ	θ	r in Au	θ	θ
− ∞	∞	45°-00'	45°-00'	∞	90°-00'	90°-00'	∞	135°-00'	135°-00'
-1000	138.42	45°-12'	44°-47'	138.42	90°-12'	89°-48'	138.42	135°-12'	134°-48'
- 100	13.85	47°-04'	42°-55'	13.85	92°-04'	87°-56'	13.85	137°-04'	132°-57'
- 75	10.40	47°-45'	42°-14'	10.39	92°-46'	87°-15'	10.39	137°-47'	132°-15'
- 50	6.94	49°-26'	40°-46'	6.94	94°-09'	85°-53'	6.94	139°-09'	130°-52'
- 25	3.50	53°-15'	36°-49'	3.50	98°-17'	81°-51'	3.49	143°-16'	126°-48'
- 10	1.48	65°-01'	25°-31'	1.47	110°-15'	70°-31'	1.46	155°-14'	115°-19'
- 7.50	1.17	70°-57'	19°-58'	1.15	116°-22'	64°-54'	1.14	161°-22'	109°-32'
- 5.00	.88	81°-10'	10°-37'	.854	127°-04'	55°-18'	.83	172°-13'	99°-32'
- 2.50	.64	100°-35'	3°-48'	.608	148°-03'	37°-28'	.57	165°-55'	80°-06'
- 1.00	.56	119°-31'	23°-39'	.519	169°-11'	20°-17'	.48	143°-26'	60°-47'

TABLE III CONTINUED

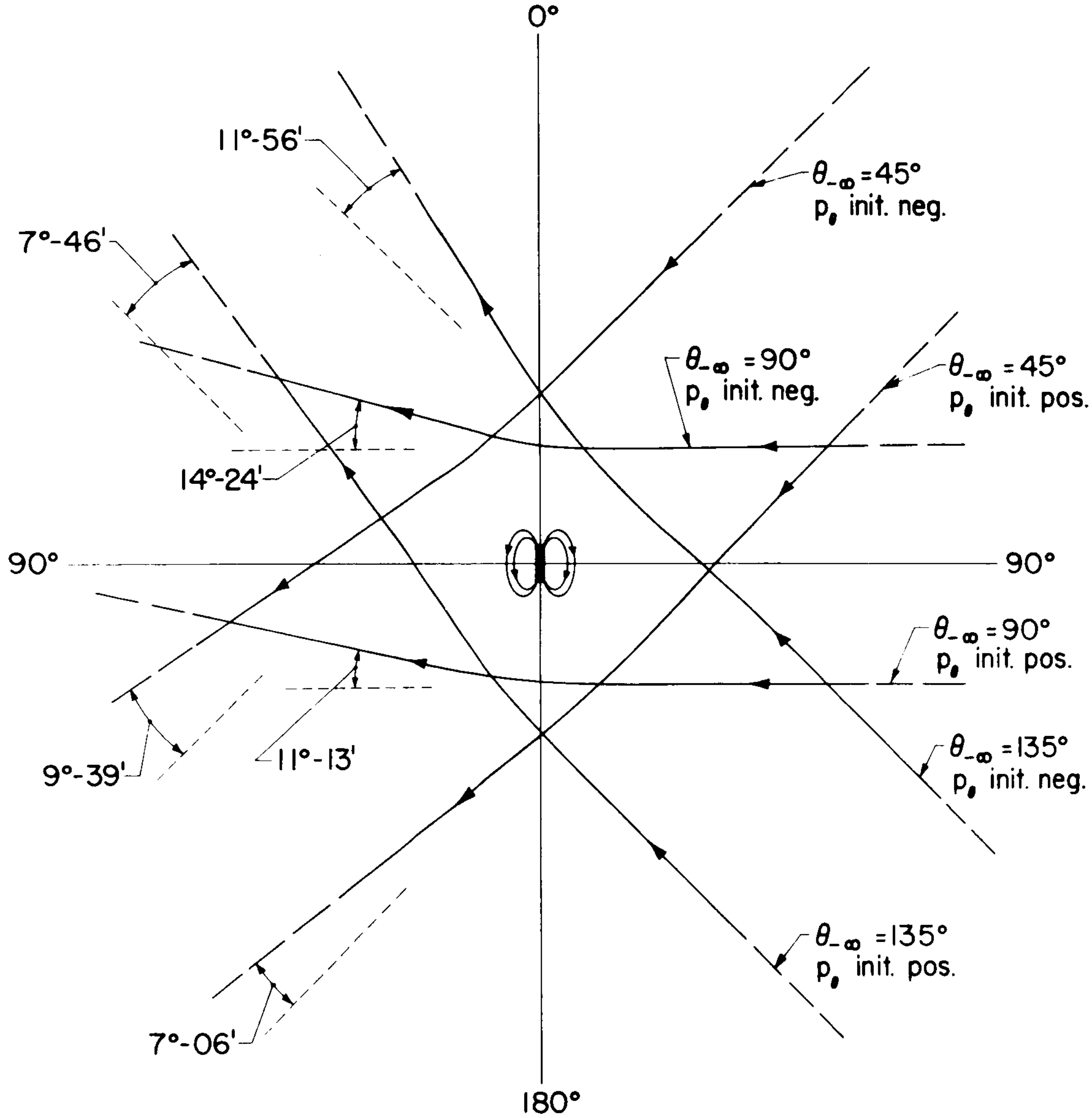
Time in 10^{-16} secs	$\theta_{-\infty} = 45°$			$\theta_{-\infty} = 90°$			$\theta_{-\infty} = 135°$		
		P_θ positive	P_θ negative		P_θ positive	P_θ negative		P_θ positive	P_θ negative
0	.54	134°-46'	36°41'	.500	173°-42'	6°-59'	.46	125°-11'	45°-24'
1.00	.56	150°-15'	50°-09'	.519	156°-41'	7°-48'	.48	107°-27'	30°-29'
2.50	.64	170°-10'	67°-34'	.608	135°-47'	24°-21'	.57	86°-54'	13°-00'
5.00	.88	168°-41'	86°-31'	.854	115°-06'	41°-52'	.83	68°-01'	4°-34'
7.50	1.17	157°-18'	97°-01'	1.15	104°-35'	51°-11'	1.14	58°-55'	12°-30'
10	1.48	150°-38'	103°-17'	1.47	98°-36'	56°-39'	1.46	53°-50'	17°-09'
25	3.50	137°-17'	116°-04'	3.50	86°-53'	67°40'	3.49	44°-01'	26°-24'
50	6.94	132°-44'	120°-33'	6.94	82°-51'	71°-35'	6.94	40°-39'	29°-40'
75	10.40	131°-03'	121°-12'	10.39	81°-29'	72°-56'	10.39	39°-31'	30°-47'
100	13.85	130°-16'	122°-59'	13.85	80°-49'	73°-35'	13.85	38°-57'	31°-21'
1000	138.42	128°-08'	125°-06'	138.42	78°-59'	75°-24'	138.42	37°-26'	32°-51'
∞	∞	127°-54'	125°-20'	∞	78°-47'	75°-35'	∞	37°-16'	33°-00'

Impact parameter b = .5Au for all cases

E = 100 electron volts

$k = 1.85 \times 10^{-18}$ esu-cm

$m = 1.67 \times 10^{-24}$ gms



Radial Scale: 0.125Å = ⊢⊣

Figure 8. Comparative Meridian Plane Orbits With p_θ Initially Positive And Negative.

Table IV displays the difference in deflection angle $\beta = (\Theta_- - \Theta_+)$, for different values of Eb^2. Figure 9 shows the variation of β with Eb^2. Both from Figures 8 and 9 one can see that the deflection angle Θ is greater for p_θ initially negative, than for p_θ initially positive. From Figure 9, one can also observe that for very large impact parameters, the deflection angles tend to be equal for p_θ initially positive or negative.

TABLE IV

Variation of $\beta = (\Theta_- - \Theta_+)$ with Eb^2 and $\theta_{-\infty}$

Eb^2 in (ev-Au^2) units	$\theta_{-\infty} = 45^\circ$			$\theta_{-\infty} = 90^\circ$			$\theta_{-\infty} = 135^\circ$		
	Θ_+	Θ_-	β	Θ_+	Θ_-	β	Θ_+	Θ_-	β
12.25	11°-43'	20°-44'	9°-01'	19°-53'	33°-45'	13°-52'	12°-12'	36°-06'	23°-54'
16.00	9°-52'	15°-34'	5°-42'	16°-15'	24° 18'	8°-03'	10°-24'	22°-17'	11°-53'
20.25	8°-20'	12°-04'	3°-44'	13°-24'	18°-23'	4°-59'	9°-06'	16°-00'	6°-54'
25.00	7°-06'	9°-39'	2°-33'	11°-13'	14°-24'	3°-11'	7°-46'	11°-56'	4°-10'
36.00	5°-18'	6°-32'	1°-14'	8°-09'	9°-35'	1°-26'	5°-45'	7°-30'	1°-45'
49.00	4°-06'	4°-43'	0°-37'	6°-08'	6°-53'	0°-45'	4°-22'	5°-12'	0°-50'
64.00	3°-14'	3°-33'	0°-19'	4°-47'	5°-10'	0°-23'	3°-24'	3°-48'	0°-24'
100.00	2°-10'	2°-14'	0°-04'	3°-06'	3°-16'	0°-10'	2°-15'	2°-19'	0°-04'

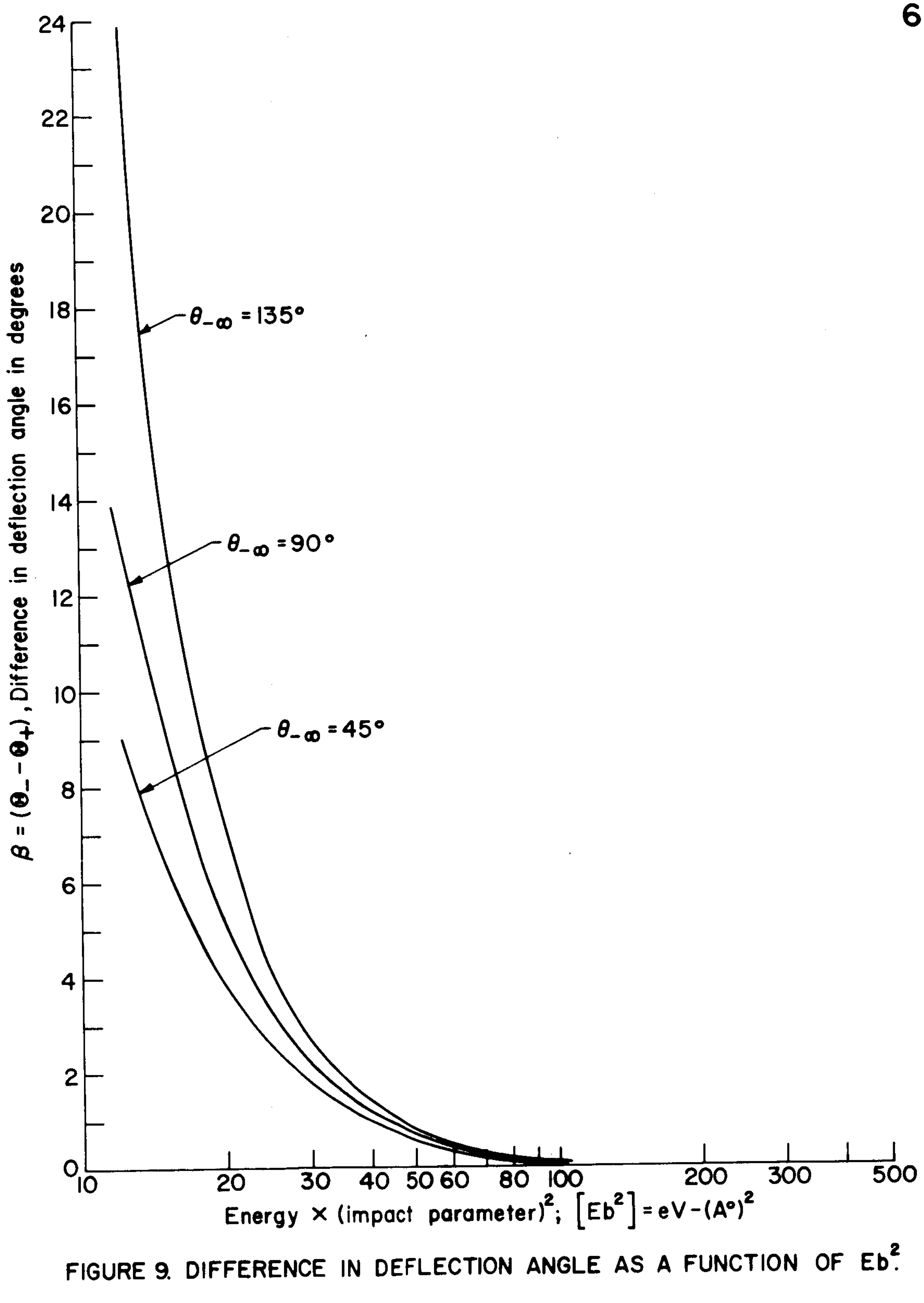


FIGURE 9. DIFFERENCE IN DEFLECTION ANGLE AS A FUNCTION OF Eb^2.

C. One Case of Non-Planar Motion:

In this section, we shall investigate the interesting case of $\alpha = p_\phi^2$ with $u_o = 0$. Then

$$f(u) = \{u^3 - \frac{\alpha}{2mke} u^2 - u\} \equiv u(u - 1)\ (u - u_3)\ ;\ u_2 = 0. \qquad (5.1)$$

where

$$u_1 = \frac{\alpha}{4mke} + \sqrt{\frac{\alpha^2}{16m^2k^2e^2} + 1}$$

and

$$u_3 = \frac{\alpha}{4mke} - \sqrt{\frac{\alpha^2}{16m^2k^2e^2} + 1}$$

From (3.8), we can write

$$u_\tau = - u_3 Sn^2 \left[\left\{ K(M) - c\ Tan^{-1} \frac{2E}{\sqrt{\alpha}} \tau \right\} /M \right] + u_3 \qquad (5.2)$$

where

$$M = \frac{-u_3}{u_1 - u_3}\ ,\ K(M) = Sn^{-1} \left\{ 1/ \quad \frac{-u_3}{u_1 - u_3} \right\}$$

and

$$c = \sqrt{\frac{mke}{2\alpha} (u_1 - u_3)}.$$

One can readily see from (5.2) that $u_\tau = u_{-\tau}$.

We can also investigate the ϕ motion for this special case. When p_ϕ is positive, from (4.35) we can write

$$\phi_{+\infty} - \phi_{-\infty} = \frac{1}{2c\,(1-u_3)} \int_{K(M)-\frac{c\pi}{2}}^{K(M)+\frac{c\pi}{2}} \frac{d\tau''}{(1 - a\mathrm{Sn}^2\tau'')} + \frac{1}{2c\,(1+u_3)} \int_{K(M)-\frac{c\pi}{2}}^{K(M)+\frac{c\pi}{2}} \frac{d\tau''}{(1 + b\mathrm{Sn}^2\tau'')} \tag{5.3}$$

where

$$a = \frac{-u_3}{1-u_3}$$

and

$$b = \frac{-u_3}{1+u_3}$$

For large impact parameters, u_3 is approximately equal to $2\,mke/\alpha$, and will be much smaller than 1 in magnitude. So we can use the Binomial approximation and write

$$\frac{1}{1 - aSn^2\tau''} \simeq 1 + aSn^2\tau'' + a^2Sn^4\tau'' \tag{5.4}$$

and

$$\frac{1}{1 + bSn^2\tau''} \simeq 1 - bSn^2\tau'' + b^2Sn^4\tau'' \quad .$$

With the above substitutions (5.3) can be reduced to

$$\phi_{+\infty} - \phi_{-\infty} = \frac{\pi}{(1 - u_3^2)} - a' \int_{K(M) - \frac{c\pi}{2}}^{K(M) + \frac{c\pi}{2}} Sn^2\tau'' d\tau'' + b' \int_{K(M) - \frac{c\pi}{2}}^{K(M) + \frac{c\pi}{2}} Sn^4\tau'' d\tau'' \quad . \tag{5.5}$$

where

$$a' = \frac{1}{c} \frac{2u_3^{\,2}}{(1 - u_3^{\,2})^2}$$

and

$$b' = \frac{1}{c} \frac{u_3^{\,2}}{(1 - u_3^{\,2})^3}$$

Since the functional parameter, M equal to $-u_3/(u_1 - u_3)$, is very small, we can write

$$\left.\begin{aligned} Sn^2\tau'' &= \sin^2\tau'' - \frac{M}{4}\,\tau''\sin 2\tau'' + \frac{M}{8}\sin^2(2\tau'') \\ &\text{and} \\ Sn^4\tau'' &= \sin^4\tau'' - M(\sin^3\tau''\cos\tau'')\tau'' - M\sin^4\tau''\cos^2\tau'' \end{aligned}\right\} \qquad (5.6)$$

where we neglect higher powers of M. Using the values given in (5.6) for $Sn^2\tau''$ and $Sn^4\tau''$ and evaluating the integral on the right side of (5.5), we finally get

$$\phi_{+\infty} - \phi_{-\infty} = \frac{\pi}{1 - u_3^2}$$

$$- a'\left[\left(\frac{1}{2} + \frac{M}{8}\right)\left(c\pi - \cos 2K(M)\sin c\pi\right) - \frac{M}{16}\cos 4K(M)\sin 2c\pi\right.$$
$$\left. + \frac{M}{8}\left\{\left(K(M) + \frac{c\pi}{2}\right)\cos\left(2K(M) + c\pi\right) - \left(K(M) - \frac{c\pi}{2}\right)\cos\left(2K(M) - c\pi\right)\right\}\right]$$

$$+ b'\left[\left(1 - \frac{M}{4}\right)\left(\frac{5}{8}c\pi - \frac{1}{2}\cos 2K(M)\sin c\pi\right)\right. \qquad (5.7)$$
$$- \frac{M}{4}\left\{\left(K(M) + \frac{c\pi}{2}\right)\sin^4\left(K(M) + \frac{c\pi}{2}\right) - \left(K(M) - \frac{c\pi}{2}\right)\sin^4\left(K(M) - \frac{c\pi}{2}\right)\right\}$$
$$\left. + \frac{M}{48}\left\{\sin^3\left(2K(M) + c\pi\right) - \sin^3\left(2K(M) - c\pi\right)\right\}\right].$$

Applying (5.7), we can calculate the difference in azimuthal angle $\gamma = (\phi_{+\infty} - \phi_{-\infty})$, for small values of u_3. Table V gives the difference for different values of u_3. We find that this difference tends to 180°, when u_3 decreases in magnitude. From table V, we can infer that this difference is most probably 180°, and that the departure from the value of 180° is most likely due to the various approximations we have made in the evaluation of the integral in (5.5). We have adopted the above method of evaluation, i.e. expanding the Sn functions in terms of sine functions and the parameter M, because exact evaluation of the integrals in (5.5) becomes difficult. For example the integral

$$I \equiv \int_{K(M) - \frac{c\pi}{2}}^{K(M) + \frac{c\pi}{2}} \mathrm{Sn}^2 \tau' \, d\tau'$$

can be evaluated* as

$$I = \frac{1}{M}\left[c\pi + \int_0^{\sin^{-1}\left\{\mathrm{Sn}\left(K(M) + \frac{c\pi}{2}\right)\right\}} \sqrt{1 - M\sin^2 \upsilon}\, d\upsilon - \int_0^{\sin^{-1}\left\{\mathrm{Sn}\left(K(M) - \frac{c\pi}{2}\right)\right\}} \sqrt{1 - M\sin^2 \upsilon}\, d\upsilon \right] \tag{5.8}$$

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*In Byrd and Friedman's "Handbook of Elliptic Integrals for Engineers and Physicists", these integrals have been evaluated in page 191. Also see page 18 of the same book.

Though

$$\text{Sn}\left[\left\{K(M)+\frac{c\pi}{2}\right\}\right]=\text{Sn}\left\{K(M)-\frac{c\pi}{2}\right\},$$

it is not clear whether the two integrals in (5.8) will cancel out.

TABLE V

Variation of γ with the Value of u_3

u_3	a	b	$\gamma^{\circ} = (\phi_{+\infty} - \phi_{-\infty})^{\circ}$
- .1926	.1615	.2385	182° - 04'
- .1623	.1396	.1937	181° - 28'
- .1231	.1096	.1404	180° - 45'

CHAPTER 6

SUMMARY AND CRITIQUE

In this Chapter, we summarize our findings and propose possible avenues of further investigation of this problem.

We have first of all demonstrated that for all $1/r^2$ potentials, irrespective of their angular dependence, the square of the radial vector is a quadratic in time.* For our specific problem, we have identified an important constant of motion, $\alpha = p_\theta^2 + (p_\phi^2/\sin^2\theta) + 2\,mke\cos\theta$, in addition to E and p_ϕ. We have also shown, that by suitable translation of the origin of time (i.e., the time $\tau = 0$ when the ion is closest to the force center) we can obtain a symmetric quadratic expression in time, $r^2 = (2E/m)\tau^2 + \alpha/2Em$.

Further, we have investigated in depth the comparatively simple case of motion in the meridian plane with a view to understanding some of the complexities of the general problem. We have expressed the polar angle θ as a function of time, by means of the Jacobian elliptic function Sn. It has been shown that the general

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*This was first demonstrated by T. D. Wilkerson (15) and independently given in a recent preprint sent to us by K. Fox (13).

meridian plane orbit can be defined in terms of three parameters: $\theta_{-\infty}$ (the asymptotic polar angle), energy E and the impact parameter $b_{-\infty}$. A few representative figures corresponding to motion in the meridian plane have been given. These figures exhibit such interesting details as the angular dependence of the orbits, the effect of the sign of initial p_θ on the orbits and deflection angles, the variation of deflection angles with $Eb^2_{-\infty}$ and finally the expected tendency for the trajectories to curve inwards in the attractive hemisphere and outwards in the repulsive hemisphere.

We have also discussed another interesting aspect of this problem, namely the turning points. We have shown that we have two types of turning points, the radial and the angular, for the dipole problem. For the case of motion in the meridian plane, we have further shown that the orbits in general cannot be reflected about apsidal vectors. (Special exceptions have been noted in Chapter 3.) We have indicated that a particularly interesting exception arises when the two turning points merge; the ion retraces its curved path after reaching the common turning point.

We have also solved the general case of non planar motion and obtained an expression for $(\phi_{+\infty} - \phi_{-\infty})$ in terms of $\Pi(u,\beta^2)$ functions which are types of incomplete elliptic integrals of the third kind. Finally we have discussed the interesting case of $\alpha = p_\phi^2$ with $u_o = 0$.

This problem can be investigated further regarding certain aspects like the effects of polarizability, finite size and rotation of the polar molecule on the trajectory of the ion. Regarding polarizability, we can regard the ion-polar molecule interaction as classical, if the sum of the Van-der Waal's radii of the ion molecule pair is less than the impact parameters of interest. Then we can write the ion molecule potential energy* as

$$V(r,\ \theta) = \frac{ke\cos\theta}{r^2} - \frac{\alpha_o e^2}{2r^4} \tag{6.1}$$

where

r = ion-molecule separation distance

θ = angle between the positive end of the dipole axis and the vector $\vec{r}$.

α_o = average electronic polarizability of the polar molecule.

We note that (6.1) presupposes that the polarizability of the polar molecule does not depend upon the relative orientation of the molecule to the $\underline{r}$ vector. (We assume that the polarization effect is isotropic). We can conclude that the effect of this altered potential energy is to cause less θ deflection of the trajectory.

As regards the second effect, namely the finite size of the dipole, we can choose elliptic coordinates** to describe the position of the ion. Thus we can define two elliptic coordinates ε, and η as shown in Figure 10,

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*J.V. Dugan, Jr. and J. L. Magee have used the above potential energy (8).

**K. Fox and J. E. Turner have analysed the bound state problem in the field of a finite dipole, using elliptic coordinates (9).

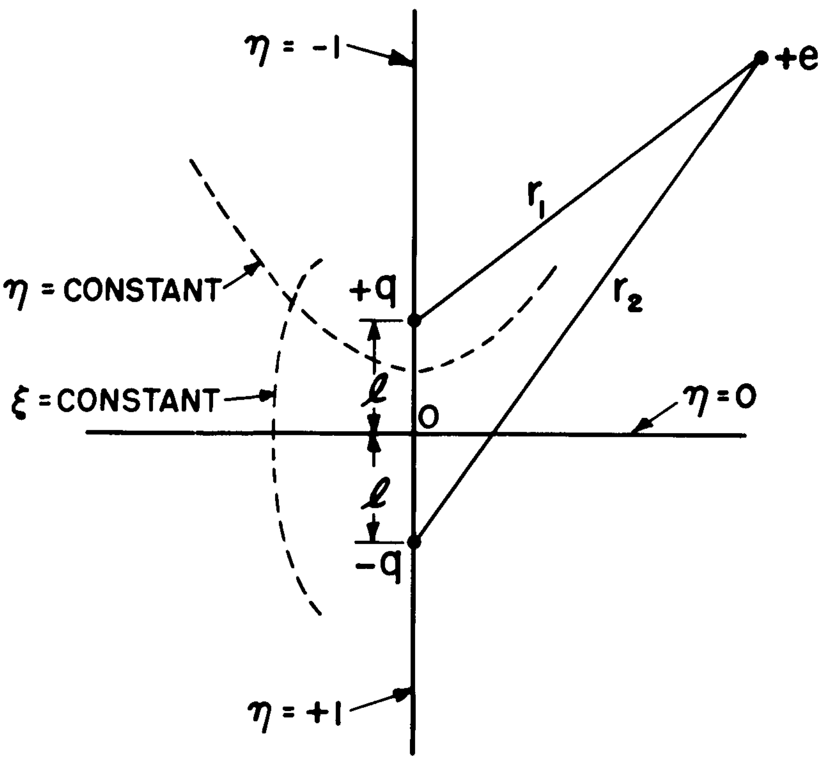


Figure 10. Elliptic Coordinate Reference System.

where

$$\varepsilon = \frac{r_1 + r_2}{2\ell} \quad ; \quad (1 \leq \varepsilon \leq \infty)$$

and

$$\eta = \frac{r_1 - r_2}{2\ell} \quad ; \quad (-1 \leq \eta \leq 1) \tag{6.2}$$

and

r_1 = distance of the ion from charge +e

and

r_2 = distance of the ion from charge -e

and

2ℓ = length of the dipole.

With these new coordinates the Hamiltonian is

$$H = \frac{1}{\varepsilon^2 - \eta^2}\left[\frac{1}{2m\ell^2}\left\langle\left(\varepsilon^2 - 1\right) p_\varepsilon^2 + (1 - \eta^2)\, p_\eta^2 + p_\phi^2\left(\frac{1}{\varepsilon^2 - 1} + \frac{1}{1 - \eta^2}\right)\right\rangle - \frac{2e^2}{\ell}\eta\right] \tag{6.3}$$

where p_ε, p_η and p_ϕ are all the momenta conjugate to the coordinates ε, η and ϕ respectively. The Hamiltonian given in (6.3) will serve as a starting point to carry out analysis of unbound ion motion in the field of finite dipole, particularly for orbits having small r_{min} ($\lesssim$ .2A°).

We can deal with the rotational effect, by noting that rotational excitation involves transfer of many quanta of rotational energy even at large impact parameters. So we can use a classical description of the molecular rotation. The rotational motion can be investigated by re-writing the Hamiltonian as

$$H = T_R + T_{ion} + V(r,\gamma)$$

where T_R, T_{ion} and $V(r,\gamma)$ are the rotational kinetic energy of the dipole, the kinetic energy of the ion and the interaction potential energy respectively. The interaction potential energy can be written as

$$V(r,\gamma) = \frac{ke \cos\gamma}{r^2} \tag{6.4}$$

where γ is the angle between the dipole axis and the radial vector of the ion and can be expressed by the following relation

$$\cos\gamma = \cos\theta \cos\theta' + \sin\theta \sin\theta' \cos(\phi - \phi') \tag{6.5}$$

θ' and ϕ' are the polar and the azimuthal angles of the dipole axis.

Let us assume for simplicity that the mass distribution of the dipole body is such that two of the principal Moments of Inertia are equal (I) and the third (about the body Z-axis) is zero. The familiar form of rotational kinetic energy thus reduces to $\frac{I}{2} (\dot{\theta}^E)^2 + (\dot{\phi}^E)^2 \sin^2 \theta^E$.

where E denotes Euler angle. Figure 11 illustrates the simple trans-formation required to then make use of the angles θ' and ϕ' employed above;

$$\theta^E = \theta'; \quad \phi^E = \pi/2 + \phi' .$$

Therefore, the rotational kinetic energy becomes

$$T_R = \frac{I}{2} \left\{ (\dot{\theta}')^2 + (\dot{\phi}')^2 \sin^2 \theta' \right\} \tag{6.6}$$

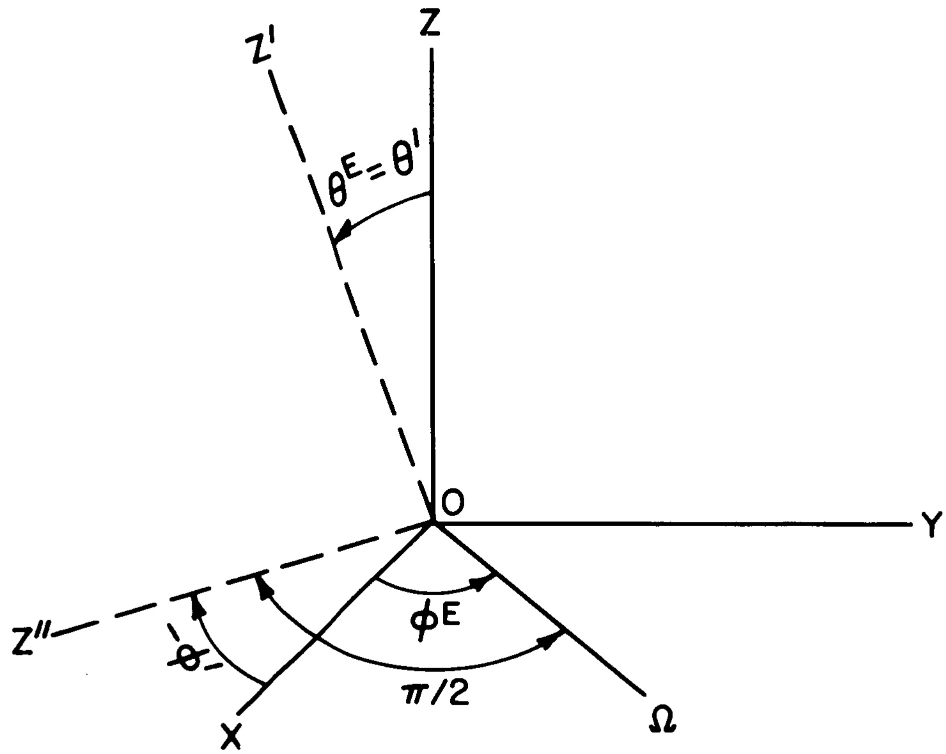


Figure II. Coordinate System Used For Consideration Of Rotational Effect.

where I is the Moment of Inertia of the dipole about any axis lying in a plane normal to the dipole axis. With T_R and $V(r,\gamma)$ known, we can write the Hamiltonian of the system comprising the ion and the dipole as

$$H = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2\sin^2\theta} + \frac{p_\theta'^2}{2I} + \frac{p_\phi'^2}{2I\sin^2\theta'} + \frac{ke}{r^2}\left\{\cos\theta\ \cos\theta' + \sin\theta\ \sin\theta'\ \cos(\phi - \phi')\right\} \tag{6.7}$$

where the primed and unprimed p's are the momenta conjugate to the primed and unprimed coordinates. We can see from (6.7) that p_ϕ is no longer conserved. It would appear that the Hamilton-Jacobi theory may prove more useful to tackle this problem.

APPENDIX A

EFFECT OF ION ENERGY ON MOLECULAR ROTATION

We can estimate the ion energy above which the rotational effect of the polar molecule can be neglected in the following way. From Figure 12a,

$$c = e\ell E \sin\theta \tag{A.1}$$

where c is the couple acting on the dipole of length ℓ due to an electric field E caused by the ion, e is the charge and θ is the angle of rotation of the dipole. The characteristic period of rotation of the polar molecule can be found, by regarding the oscillation to involve small angle only. Since

$$c = I\frac{d^2\theta}{dt^2} \tag{A.2}$$

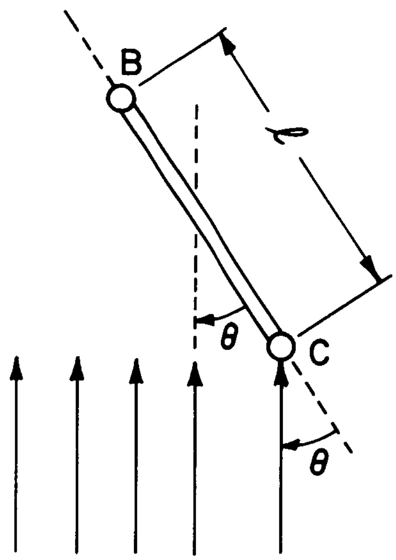
where I is the Moment of Inertia of the polar molecule about its axis of rotation, we have from (A.1) and (A.2)

$$\frac{d^2\theta}{dt^2} + \frac{e\ell E}{I}\theta = 0 \tag{A.3}$$

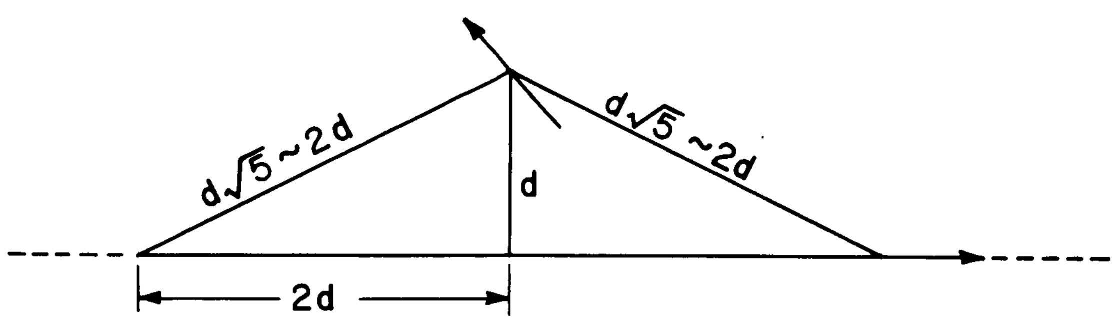
whence the natural period P is given as

$$P = \sqrt{\frac{4\pi^2 I}{e\ell E}} \tag{A.4}$$

From the figures of the orbits that we have drawn, we note that the deflection of the ion from a nearly straight line trajectory starts practically when the ion is at a distance of 1.5 times the minimum distance r_{min} from the force center. So we can regard a distance



(a). Couple Acting On The Polar Molecule.
Field Lines Rougly Parallel From Ion.



(b). Classical Path Of The Ion.

FIGURE 12. ROTATIONAL EFFECT OF THE POLAR MOLECULE.

equal to $2r_{min}$ as the effective range of E. (The electric field will be down to a fourth of its maximum value, when the ion is at $2r_{min}$.) We can calculate P by substituting an average value of E in (A.4).

$$E_{average} \simeq \frac{e}{2r_{min}^2} \; .$$

$$\therefore \quad P \simeq \sqrt{\frac{8\pi^2 I r_{min}^2}{e^2 \ell}} \qquad (A.5)$$

The classical period of action is given by τ, where

$$\tau \simeq \frac{4r_{min}}{v} \; ; \quad v \text{ is the velocity of the ion.}$$

So we get

$$\frac{P}{\tau} \simeq v \sqrt{\frac{\pi^2 I}{2e^2 \ell}} \qquad (A.6)$$

Moment of Inertia of the water molecule is I, where

$$I \sim 1 \text{ to } 3 \times 10^{-40} \text{ gms - cm}^2 \; .$$

The factor $e^2 \ell$ is roughly about 25×10^{-28}. So we get

$$\frac{P}{\tau} \simeq (6.5 \times 10^{-1}) v \qquad (A.7)$$

Since the velocity v is $\sqrt{2E/m}$, we can calculate the ratio $\frac{P}{\tau}$ for ions of different energy. Table 6 gives the value of $\frac{P/2}{\tau}$ for ions of different energy. The ratio $\frac{P/2}{\tau}$ can be regarded as a measure of the applicability of our formulation. The higher this ratio, the greater is the justification for neglecting the rotational effect of the polar molecule. Thus our calculations are well founded for kilovolt protons in a molecular dipole field of this strength, while molecular rotation would surely have to be considered for proton energies of 10eV and below.

TABLE VI

Ratio of Semi-Natural Period of Rotation to Classical Time of Action

v in cms	Energy of the ion in e.v.	$\frac{P/2}{\tau}$
4.5×10^7	1000	~ 15
1.4×10^7	100	~ 4.5
$.45 \times 10^7$	10	~ 1.5

APPENDIX B

ELLIPTIC FUNCTIONS

We note the equivalence of the integrals

$$u = \int_o^x \frac{dt}{\left\{(1 - t^2)(1 - Mt^2)\right\}^{1/2}} = \int_o^\phi \frac{d\theta}{(1 - M\,\mathrm{Sin}^2\,\theta)^{1/2}} \qquad \text{(B.1)}$$

where

$$t = \sin\theta, \quad x = \sin\phi.$$

The Jacobian elliptic functions can be defined by the relations

$$\mathrm{Sn}\,u = \sin\phi, \quad \mathrm{cn}\,u = \cos\phi, \quad \mathrm{dn}\,u = (1 - M\sin^2\phi)^{1/2}$$

or equivalently

$$\mathrm{Sn}\,u = x, \quad \mathrm{cn}\,u = (1 - x^2)^{1/2}, \quad \mathrm{dn}\,u = (1 - M\,x^2)^{1/2}$$

where the positive square root is to be taken in every case. Here u and M are known as the argument and the functional parameter respectively. There is also the complementary parameter M_1, defined as $(1 - M)$. As we have mentioned earlier, it is customary to write these functions as $\mathrm{Sn}(u/M)$, $\mathrm{cn}(u/M)$ and $\mathrm{dn}(u/M)$ with a stroke separating the argument and the functional parameter. The three Jacobian elliptic functions are single-valued functions of the argument u and are doubly periodic. We have also two other quantities called K(M) and K'(M) defined by the relations,

$$K(M) = \int_0^{\frac{\Pi}{2}} \frac{d\theta}{(1 - M\sin^2\theta)^{1/2}} \; ; \quad iK'(M) = i\int_0^{\frac{\Pi}{2}} \frac{d\theta}{(1 - M_1\sin^2\theta)^{1/2}} \tag{B.2}$$

These are the real and imaginary quarter periods.

We list some of the important properties of these functions which we have used elsewhere.

$$\left.\begin{aligned}
&\text{Sn}\,(u/o) = \sin u, \quad \text{cn}\,(u/o) = \cos u, \quad \text{dn}\,(u/o) = 1. \\
&\text{Sn}\,(u/1) = \tanh u, \quad \text{cn}\,(u/o) = \text{dn}\,(u/1) = \text{sech}\; u. \\
&\text{Sn}\,(-u) = -\,\text{Sn}\,u. \\
&\text{Sn}\,\{2K(M) - u\} = \text{Sn}\,u \\
&\text{Sn}\,u = \frac{\text{cn}\{K(M)-u\}}{\text{dn}\{K(M)-u\}} \\
&\text{Sn}(u/M) = \sin u - \frac{1}{4} M \cos u\,(u - \sin u \cos u)\;;\quad M \text{ very small}
\end{aligned}\right\} \tag{B.3}$$

Now we shall show that irrespective of the change in sign of $\underline{p_\theta}$ during motion, the expression for u_τ will depend only on the sign of initial $\underline{p_\theta}$.

<u>Case 1</u> p_θ is initially positive. Let us evaluate u_τ at some time τ, such that $\tau < \tau_3$. Then p_θ will always remain positive. We have already seen in Chapter 3, that we have to evaluate the integral I,

where

$$I = \int \mp \frac{du}{\sqrt{2\ mke}\ \sqrt{f(u)}}$$

and the negative sign should be taken when p_θ is positive, and the positive sign when p_θ is negative. So we have

$$\int_{u_{-\infty}}^{u_\tau} \frac{-du}{\sqrt{2\ mke}\ \sqrt{f(u)}} = \frac{1}{\sqrt{\alpha}} \{\frac{\pi}{2} + \mathrm{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau\},$$

which can be rewritten as

$$\int_{u_3}^{u_{-\infty}} \frac{du}{\sqrt{2\ mke}\ \sqrt{f(u)}} - \int_{u_3}^{u_\tau} \frac{du}{\sqrt{2\ mke}\ \sqrt{f(u)}} = \frac{1}{\sqrt{\alpha}} \{\frac{\pi}{2} + \tan^{-1} \frac{2E}{\sqrt{\alpha}} \tau\};$$

whence

$$u_\tau = (u_2 - u_3)\ \mathrm{Sn}^2 \{(\delta - c\beta)\} + u_3, \tag{B.4}$$

where

$$\delta = \mathrm{Sn}^{-1} \left\{\left(\frac{u_{-\infty} - u_3}{u_2 - u_3}\right)\right\}^{1/2} \Big/ M \ ; \ M = \frac{u_2 - u_3}{u_1 - u_3}$$

and

$$\beta = \{\frac{\pi}{2} + \mathrm{Tan}^{-1} \frac{2E}{\sqrt{\alpha}} \tau\}$$

and

$$c = \sqrt{\frac{mke\ (u_1 - u_3)}{2\alpha}}$$

Let us evaluate u_τ at time $\tau > \tau_3$. Now p_θ will remain positive until u_3 is reached, and afterwards negative. So we have

$$\int_{u_{-\infty}}^{u_3} \frac{-du}{\sqrt{2mke}\ \sqrt{f(u)}} + \int_{u_3}^{u_\tau} \frac{du}{\sqrt{2mke}\ \sqrt{f(u)}} \tag{B.5}$$

$$= \frac{1}{\sqrt{\alpha}} \left\{ \frac{\pi}{2} + \tan^{-1} \frac{2E}{\sqrt{\alpha}}\, \tau \right\}$$

where we have reversed the sign of the second integral, to account for the change in sign of p_θ after u_3 is reached. (B.5) can be solved to yield

$$u_\tau = (u_2 - u_3)\ Sn^2\ (c\beta - \delta) + u_3 \tag{B.6}$$

As $Sn(-u)$ is equal to $-Sn(u)$, we note that

$$(u_2 - u_3) Sn^2\ (c\beta - \delta) + u_3 \equiv (u_2 - u_3)\ Sn^2 (\delta - c\beta) + u_3$$

Let us next evaluate u_τ at time τ, such that

$$\tau_3 < \tau_2 < \tau.$$

This means that p_θ will be positive from $u_{-\infty}$ to u_3, negative from

u_3 to u_2, and again positive from u_2 to u_τ. So we have

$$\frac{1}{(2mke)^{1/2}}\left[\int_{u_{-\infty}}^{u_3} \frac{-du}{\sqrt{f(u)}} + \int_{u_3}^{u_2} \frac{du}{\sqrt{f(u)}} - \int_{u_2}^{u_\tau} \frac{du}{\sqrt{f(u)}}\right]$$

$$= \frac{1}{\sqrt{\alpha}}\left(\frac{\pi}{2} + \mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\,\tau\right) \tag{B.7}$$

This can be rewritten as

$$\frac{1}{(2mke)^{1/2}}\left[\int_{u_3}^{u_{-\infty}} \frac{du}{\sqrt{f(u)}} + \int_{u_3}^{u_2} \frac{du}{\sqrt{f(u)}} + \int_{u_3}^{u_2} \frac{du}{\sqrt{f(u)}} - \int_{u_3}^{u_\tau} \frac{du}{\sqrt{f(u)}}\right]$$

$$= \frac{1}{\sqrt{\alpha}}\left(\frac{\pi}{2} + \mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\,\tau\right)$$

Since

$$\int_{u_3}^{u_2} \frac{du}{\sqrt{f(u)}} = \frac{2}{(u_1 - u_3)^{1/2}}\,K(M),$$

(B.7) reduces to

$$\delta + 2K(M) - \mathrm{Sn}^{-1}\left\{\left(\frac{u - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\} = c\left(\frac{\pi}{2} + \mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\,\tau\right)$$

whence

$$u_\tau = (u_2 - u_3)\, Sn^2 \{ 2\, K(M) + (\delta - c\beta)\} + u_3 , \qquad (B.8)$$

which can be still further reduced to

$$u_\tau = (u_2 - u_3)\, Sn^2 (\delta - c\beta) + u_3 \quad .$$

Thus we see that when p_θ is initially positive, we always get

$$u_\tau = (u_2 - u_3)\, Sn^2 \left[Sn^{-1} \left\langle \left(\frac{u_{-\infty} - u_3}{u_2 - u_3} \right)^{1/2} \Big/ M \right\rangle - c \left\{ \frac{\Pi}{2} + Tan^{-1} \frac{2E}{\sqrt{\alpha}} \tau \right\} \right] + u_3$$

Case 2

We can show that the expression for u_τ will remain unaffected, for the other case i.e., p_θ initially negative also.

Let us first evaluate u_τ at time τ, with $\tau < \tau_2$. As p_θ will always remain negative, we write

$$\int_{u_{-\infty}}^{u_\tau} \frac{du}{\sqrt{2mke}\,\sqrt{f(u)}} = \frac{1}{\sqrt{\alpha}} \{ \frac{\pi}{2} + Tan^{-1} \frac{2E}{\sqrt{\alpha}} \tau \}$$

Rewriting the above equation as

$$\int_{u_3}^{u_\tau} \frac{du}{\sqrt{2mke}\,\sqrt{f(u)}} - \int_{u_3}^{u_{-\infty}} \frac{du}{\sqrt{2mke}\,\sqrt{f(u)}} = \frac{1}{\sqrt{\alpha}}\ \beta \ .$$

we find

$$u_\tau = (u_2 - u_3)\,\mathrm{Sn}^2\{\delta + c\beta\} + u_3 \quad . \tag{B.9}$$

Let us finally consider that

$$\tau_2 < \tau_3 < \tau.$$

For this case p_θ will be negative at first, until u_2 is reached, then positive until u_3 is reached, and then once again negative until u_τ is reached. So we have

$$\frac{1}{(2mke)^{1/2}}\left[\int_{u_{-\infty}}^{u_2}\frac{du}{\sqrt{f(u)}} - \int_{u_2}^{u_3}\frac{du}{\sqrt{f(u)}} + \int_{u_3}^{u_\tau}\frac{du}{\sqrt{f(u)}}\right] = \frac{1}{\sqrt{\alpha}}\,\beta \quad . \tag{B.10}$$

Rewriting the above equation, we get

$$\frac{1}{(2mke)^{1/2}}\left[-\int_{u_3}^{u_{-\infty}}\frac{du}{\sqrt{f(u)}} + \int_{u_3}^{u_2}\frac{du}{\sqrt{f(u)}} + \int_{u_3}^{u_2}\frac{du}{\sqrt{f(u)}} + \int_{u_3}^{u_\tau}\frac{du}{\sqrt{f(u)}}\right]$$

$$= \frac{1}{\sqrt{\alpha}}\,\beta \ .$$

Whence

$$-\,\delta + 2\,K(M) + \mathrm{Sn}^{-1}\left\{\left(\frac{u_\tau - u_3}{u_2 - u_3}\right)^{1/2}\Big/ M\right\} = c\beta$$

So we finally write

$$u_\tau = (u_2 - u_3)\ \mathrm{Sn}^2\{\delta + c\beta - 2K(M)\} + u_3 \tag{B.11}$$

which can be reduced to

$$u_\tau = (u_2 - u_3)\ \mathrm{Sn}^2\ (\delta + c\beta) + u_3 \ .$$

Thus we see that when p_θ is initially negative, we always get

$$u_\tau = (u_2 - u_3)\ \mathrm{Sn}^2\left[\mathrm{Sn}^{-1}\left\{\left(\frac{u_{-\infty} - u_3}{u_2 - u_3}\right)^{1/2} \Big/ M\right\} + c\left\{\frac{\pi}{2} + \mathrm{Tan}^{-1}\frac{2E}{\sqrt{\alpha}}\,\tau\right\}\right] + u_3 \ .$$

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