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QUALITATIVE COMPUTER STUDIES OF NEW n-BODY MODELS OF ATOMS AND MOLECULES: PRELIMINARY REPORT

by

Donald Greenspan

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We initiate in this first of a series of papers a new computer oriented approach to the modeling of atoms and molecules. Electron-electron charge interactions are included and several qualitative computations of electron and proton motions are described. The long range goals are to describe electron configurations from nucleon configurations, to develop a viable model of the covalent bond, and to apply the resulting understanding of physical and chemical mechanisms to the study of living cell phenomena.

Qualitative Computer Studies of New n-Body Models of Atoms and Molecules: Preliminary Report

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We initiate in this first of a series of papers a new computer oriented approach to the modeling of atoms and molecules. Electron-electron charge interactions are included and several qualitative computations of electron and proton motions are described. The long range goals are to describe electron configurations from nucleon configurations, to develop a viable model of the covalent bond, and to apply the resulting understanding of physical and chemical mechanisms to the study of living cell phenomena.

1. Introduction

In our general quest to understand atomic and molecular behavior, and, in consequence, chemical, physical and biological phenomena, quantum mechanics has proved to be superior to all other theories (see, e.g., refs. [1-10, 13-17] and the numerous additional references contained therein). Yet, even this sophisticated mathematical approach has glaring deficiencies, as, for example, those relating to incorrect predictions of molecular bond angles and various nuclear energies [6, 7, 15, 16]. Some of these problems result from the lack of knowledge of nuclear structure and nuclear potentials [7], while others, for example, arise from the simplistic assumption that one-electron orbital results can be extrapolated to larger atoms and to molecules, thereby neglecting electron-electron charge and spin interactions [6, 15]. From the dynamical point of view, the prohibitive number of dimensions required by the quantum mechanical approach, even for the three-body problem [5, 8-10], renders the approach completely impractical for the study of all phenomena which involve the interactions of relatively large numbers of particles [11].

For all the reasons listed above, we will initiate here a new computer oriented approach to the study of atoms and molecules. Our present examples will be largely qualitative, but will allow for electron-electron charge interactions. Without doubt, we will present many more questions than answers, but those few answers to be given will be most interesting, since our formulation will be completely deterministic and yet possess certain basic characteristics in common with results of quantum mechanics. The enhancement of the present models and possible courses for future research will be discussed in the final section.

2. Mathematical Preliminaries

Let us first give the precise description of an explicit, computer oriented, recursive method for solving an n-body problem. For positive time step Δt, let $t_k = k\Delta t$, $k = 0,1,2,\ldots$. For $i = 1,2,..,N$, let particle P_i have mass m_i and charge e_i , and at time t_k let P_i be located at $\vec{r}_{i,k}$, have velocity $\vec{v}_{i,k}$, and have acceleration $\vec{a}_{i,k}$. Let position, velocity and acceleration be related by the "leap-frog" formulas ([11], p. 107):

$$\vec{v}_{i,\frac{1}{2}} = \vec{v}_{i,0} + \frac{\Delta t}{2}\vec{a}_{i,0} \tag{2.1}$$

$$\vec{v}_{i,k+\frac{1}{2}} = \vec{v}_{i,k-\frac{1}{2}} + (\Delta t)\,\vec{a}_{i,k} \qquad , k = 1,2,\ldots. \tag{2.2}$$

$$\vec{r}_{i,k+1} = \vec{r}_{i,k} + (\Delta t)\,\vec{v}_{i,k+\frac{1}{2}} \qquad , k = 0,1,2,\ldots \; . \tag{2.3}$$

If $\vec{F}_{i,k}$ is the force acting on P_i at time t_k , then for the present we assume that force and acceleration are related by

$$\vec{F}_{i,k} = m_i\,\vec{a}_{i,k} \tag{2.4}$$

Once an exact structure is given to $\vec{F}_{i,k}$, then the motion of each particle will be determined recursively and explicitly by (2.1)-(2.4) from prescribed initial data.

The formulation (2.1)-(2.4) is economical, though only approximately conservative. Exact conservation of energy and momentum can be achieved [11], but only through an implicit, less economical approach. Throughout,

in both the two and three dimensional examples to be discussed, the time step to be used in (2.1)-(2.3) will be $\Delta t = 10^{-4}$ and a comprehensive FORTRAN program for implementation of the method is given in the Appendix of [12].

3. Physical Preliminaries

Fundamental to the models to be developed is the question of why the electron in the H atom does not fall into the nucleus. In quantum mechanics, which is strictly a descriptive theory, it is merely shown that electron capture by the nucleus would violate the uncertainty principle, and hence is not consistent with the theory [9]. However, it will be convenient, dynamically, to assume simply that "near" the nuclear surface, the electron is repelled. Thus, in addition to "long range" $\frac{1}{r^2}$ Coulomb attraction, we will allow for "short range" $\frac{1}{r^p}$ repulsion ($p > 2$) between the nucleus and the electron. Indeed, such repulsive forces are known to exist in ionic bonds, with p in the range $9 \leq p \leq 12$ [15, p. 104]. Thus, we assume that the magnitude F of the force $\vec{F}$ between the electron and the nucleus is given by

$$F = \frac{\alpha}{r^2} + \frac{\beta}{r^p}, \quad p > 2, \tag{3.1}$$

where the parameters α and β will be described in the next section. For electron-electron and proton-proton interactions, we will consider only Coulomb repulsion, which is implemented by setting $\beta = 0$ in (3.1).

4. A "Hydrogen" Atom

Let us begin by considering an atom which consists of exactly one electron and exactly one proton. We will concentrate at present only on its base state, about more which will be stated later, and will model it in a simplistic fashion which is qualitatively similiar to the H atom.

Let P_1 be the proton and P_2 the electron. Choose (3.1) to have the particular form

$$(4.1) \qquad F = \frac{e_1 e_2}{r^2} + \frac{m_1 m_2}{r^p} \quad , p > 2 \quad .$$

In analogy with hydrogen, set $m_1 = 1600$, $m_2 = 1$. For computational convenience, set $e_1 = 40$, $e_2 = -40$, since now, independently of p , the equilibrium distance between the proton and the electron is unity, because $F \equiv 0$ when $r = 1$. Finally, for later convenience, set $p = 9$, so that (4.1) takes the final form

$$(4.1) \qquad F = -\frac{1600}{r^2} + \frac{1600}{r^9} \quad .$$

Now, the probability that the electron is exactly one unit from the proton and has $\vec{0}$ velocity relative to the proton is zero, so, let us examine the motion of an electron whose distance to the proton is close to unity and whose relative velocity is nonzero. For economy, the discussion of this section is now restricted to two dimensions. To emphasize the nature of the motion, set $\vec{r}_{1,0} = \vec{v}_{i,0} = 0$, $\vec{r}_{2,0} = (1.1, 0)$, $\vec{v}_{2,0} = (0,4)$, so that the speed of P_2 is relatively large. Figure 1 shows the electron motion up to t_{15000} . This motion is orbital and consists of periodic waves which oscillate about the unit circle with an approximate period of 1.4750 seconds. (Because this paper is largely qualitative, no attempt was made to introduce the de Broglie assumption that each complete orbit consists of an integral number of half-periods). Though Figure 1 emphasizes the nature of the electron's motion in a relatively small computer time, nevertheless, for any $v_{2,0,y} \neq 0$, the qualitative character of the resulting motion was exactly the same as that shown in Figure 1. The only significant change was in wave periodicity.

Figure 2 shows the electron's position every 500 time steps up to t_{176750}, which is approximately twelve full orbits, for the same initial data as that used for Figure 1. The result is qualitatively analogous to a quantum mechanical electron cloud configuration.

It is perhaps worth noting that, again, because of the qualitative nature of our approach, we will make no special effort at energy analysis, which will be deferred to later papers.

5. A "Hydrogen" Molecule

Before proceeding to the consideration of more complex atoms, let us consider the most simple type of molecule of broad general interest, a "hydrogen type" molecule. We will do this by exploring how two atoms of the type described in Section 4 can unite as a bonded unit. Recall that the radius of the hydrogen atom is 0.53 A and the distance between the protons of the hydrogen molecule is 0.74 A. In analogy, then, with hydrogen, itself, we will try to construct our molecule so that the distance between the protons is 1.5, since the radius of the atom described in Section 4 is unity. To do this, begin again with (4.1), allowing p to be a parameter. Let P_1 and P_3 be protons and P_2 and P_4 be electrons, as shown in Figure 3, and let the initial data be $x_{1,0} = -0.75$, $y_{1,0} = 0.0$, $x_{2,0} = 0.0$, $y_{2,0} = -0.75$, $x_{3,0} = 0.75$, $y_{3,0} = 0.0$, $x_{4,0} = 0.0$, $y_{4,0} = 0.75$, $v_{i,0,x} \equiv v_{i,0,y} \equiv 0$, $i \equiv 1,2,3,4$. We now vary p from 3 - 11 to see which value then results in a molecular bond. The best such value is $p = 9$, which, incidentally, is why this choice was made in (4.2). For $p = 9$, the electrons and the protons each show only small oscillations in place. The maximum proton oscillation from its initial position was 0.0052, while each electron oscillated exceptionally rapidly with respect to each proton, but only up to a maximum distance 0.0088 from its initial

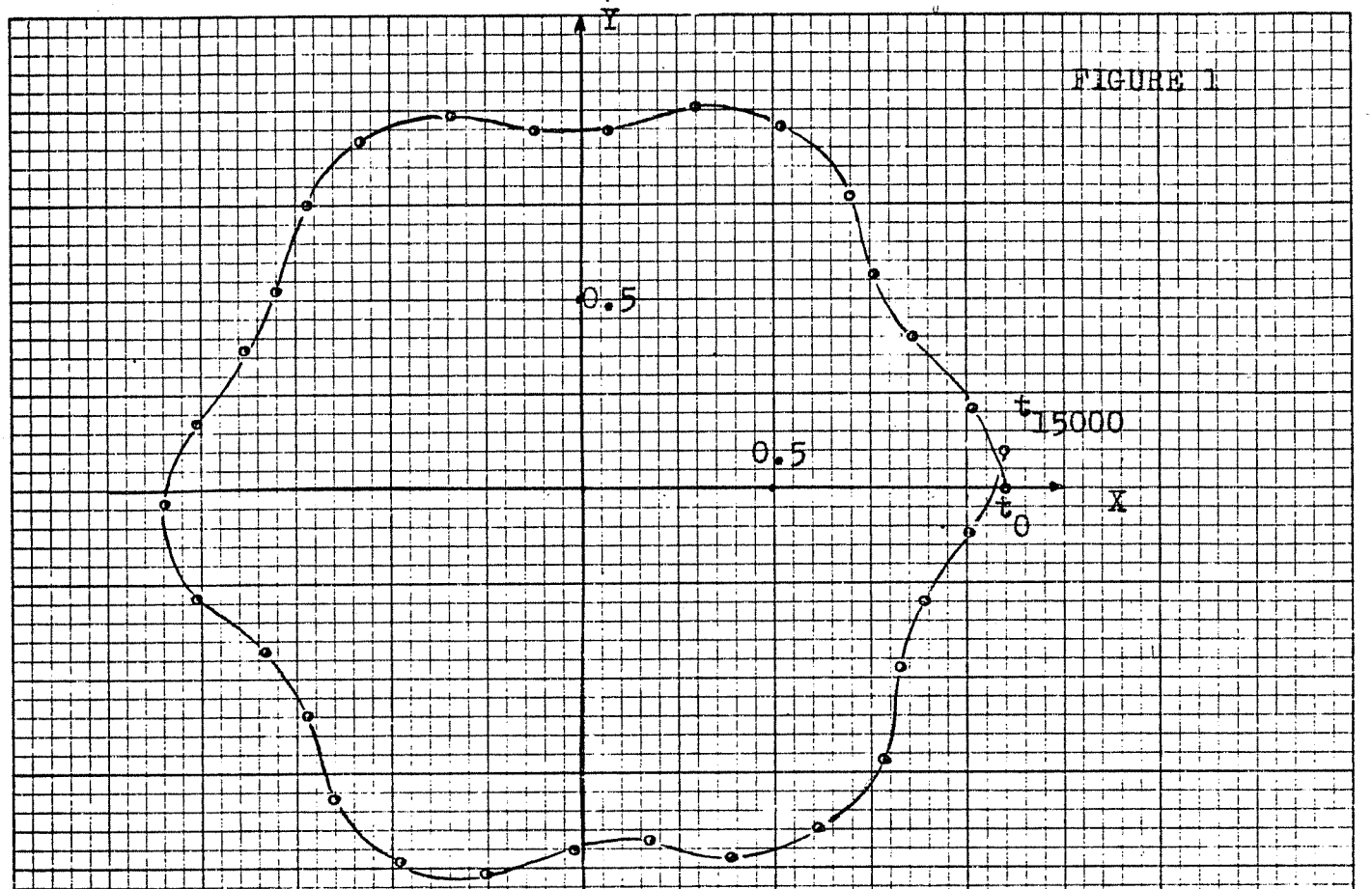


FIGURE 1

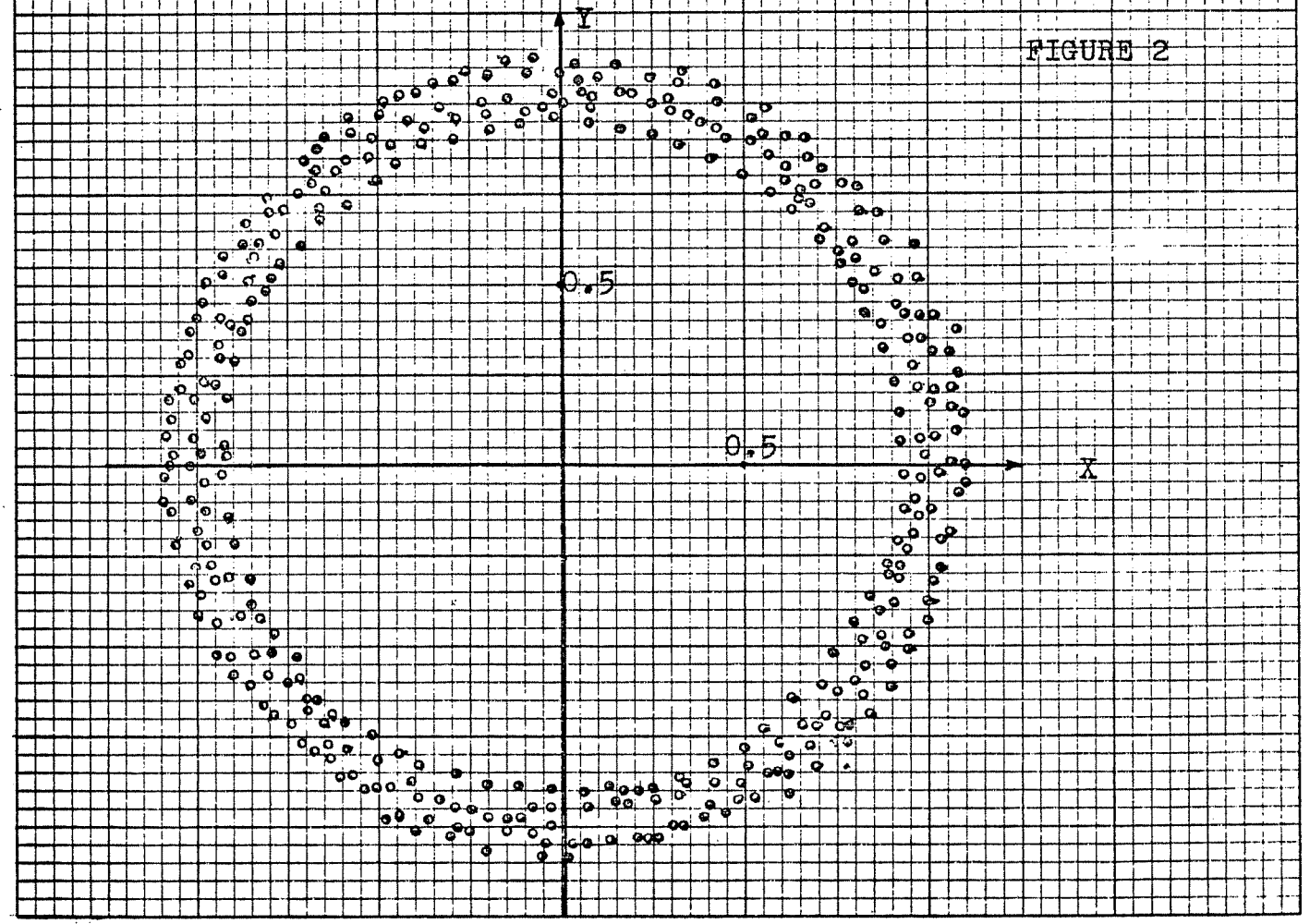


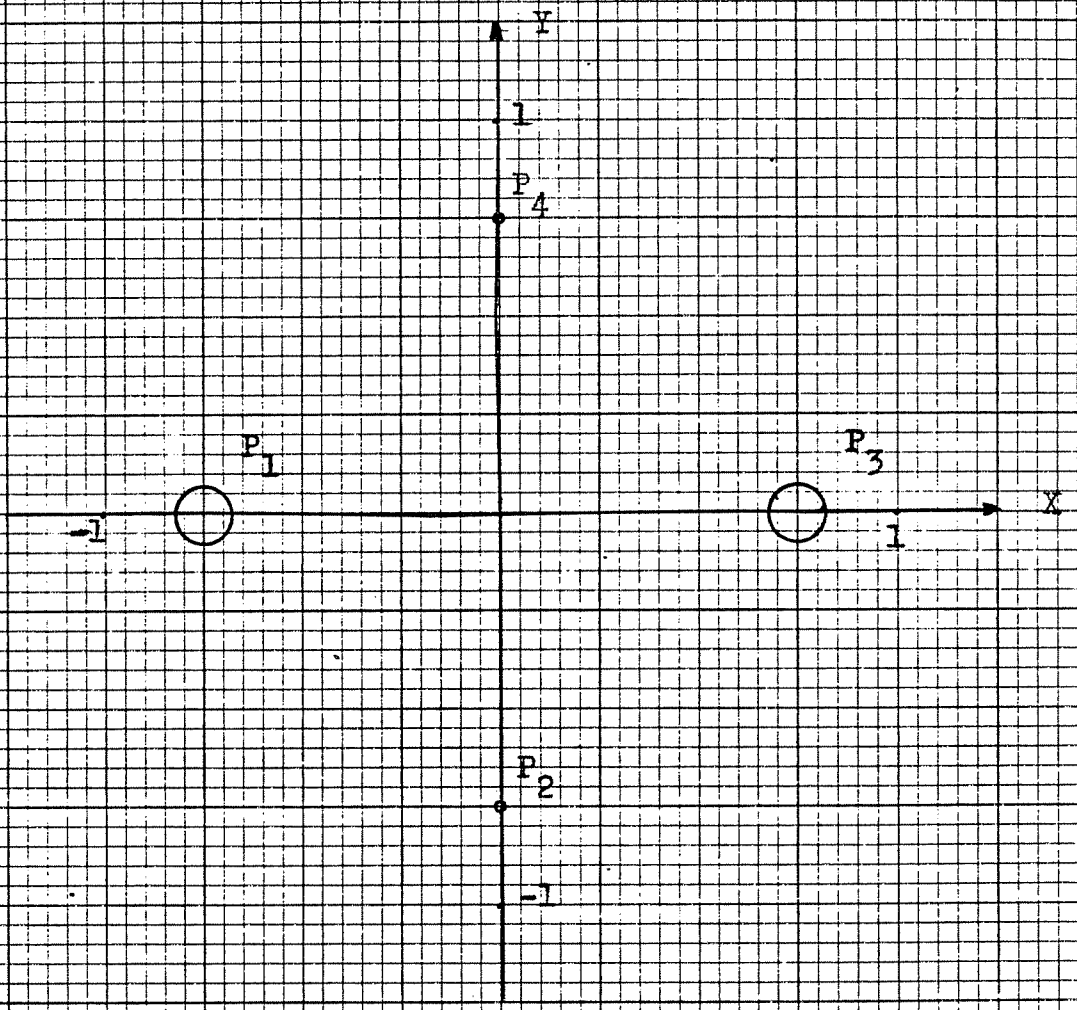
FIGURE 2

position. Small perturbations of initial electron positions did not disturb the equilibrium of the molecule. However, larger perturbations of the positions of both electrons, like resetting P_4 at (0.75, -1) and P_3 at (-0.75, 1) resulted in the dissolution of the molecule, with each separate atom drifting outward. Thus, qualitatively, the addition of a sufficient amount of energy to the molecule will result in its dissolution. Conversely, the formation of the molecule from two suitably situated atoms must result in the release of energy.

The parameter choice p = 10 yielded results which were analogous, but not quite as stable as for p = 9. All choices other than 9 or 10 in the range $3 \leq p \leq 11$ resulted in an unstable configuration in which the two atoms drifted apart.

We explore next the way in which the molecule forms by bringing two atoms close to each other in a sequence of steps. To do this, let P_1 and P_3 be the two protons, P_2 and P_4 the two electrons, and let the initial data be $x_{1,0} = -0.95$, $y_{1,0} = 0$, $x_{2,0} = -0.95$, $y_{2,0} = 1.0$, $x_{3,0} = 0.95$, $y_{3,0} = 0$, $x_{4,0} = 0.95$, $y_{4,0} = -1.0$, $v_{1,0,x} \equiv v_{i,0,y} \equiv 0$, i = 1,2, 3,4. The protons are kept fixed and only the electron motion is observed. This is shown every 500 time steps up to t_{10000} in Figure 4 (a), where, because of the symmetry of the electron motions about the origin, only the motion of P_2 is shown. Next, the protons are reset to (-0.85,0) and (0.85,0), while the electrons are taken at their final positions in Figure 4 (a), that is, at (-0.31, 1.02) and (0.31,-1.02). All initial velocities are set to $\vec{0}$ and the electron motions are shown for another 10000 time steps in Figure 4 (b). In Figure 4 (c) are shown electron motions for 10000 time steps after resetting the protons to (-0.8,0) , (0.8,0) , and taking initial electron positions as the terminal ones in Figure 4 (b),

FIGURE 3



that is (0.12, 0.64) and (-0.12, -0.64). All initial velocities again were reset to $\vec{0}$. Figure 4 (d) shows 10000 time steps of electron motion after fixing the protons at (-0.75.0), (0.75.0) and the electrons at their final positions in Figure 4 (c), that is, at (-0.15, 0.75) and (0.15, -0.75) . All initial velocities were set to $\vec{0}$. Finally, in Figure 4 (e), the protons were allowed to move freely and the electron motion is shown from their final positions of Figure 4 (d) , that is, (0.05, 0.8) and (-0.05, -0.8) . After 10000 time steps the new proton positions are shown as the dotted circles in Figure 4 (e).

From Figures 4 (a)-(e), it should be observed that the areas of electron oscillation become increasingly constrained and smaller as the protons move closer to each other. Moreover, the x-coordinates of the electrons are always between the x coordinates of the protons.

Other choices of p never gave results as satisfactory as those just described. For example, consider, at the lower extreme, p = 3. A molecule does result when the proton positions are (-1.1,0), (1.1,0) and the electron positions are (0,-1.1), (0,1.1). Small perturbations of the electrons in the Y direction only do not disturb the equilibrium of the molecule, but, invariably, perturbation of electron positions in the X-direction led to dissolution into separate atoms. Computations revealed that such perturbations resulted in electron motions in which the X-coordinates of the electrons exceeded, in absolute value, the X-coordinates of the protons. In such cases, it is indeed unrealistic to say that the $\frac{1}{r^2}$ component of force is "long range" while the $\frac{1}{r^3}$ component is "short range", since the orders of magnitudes of these quantities differ only negligibly. Thus, the choice p = 9 was, in fact, both physically and computationally a realistic one.

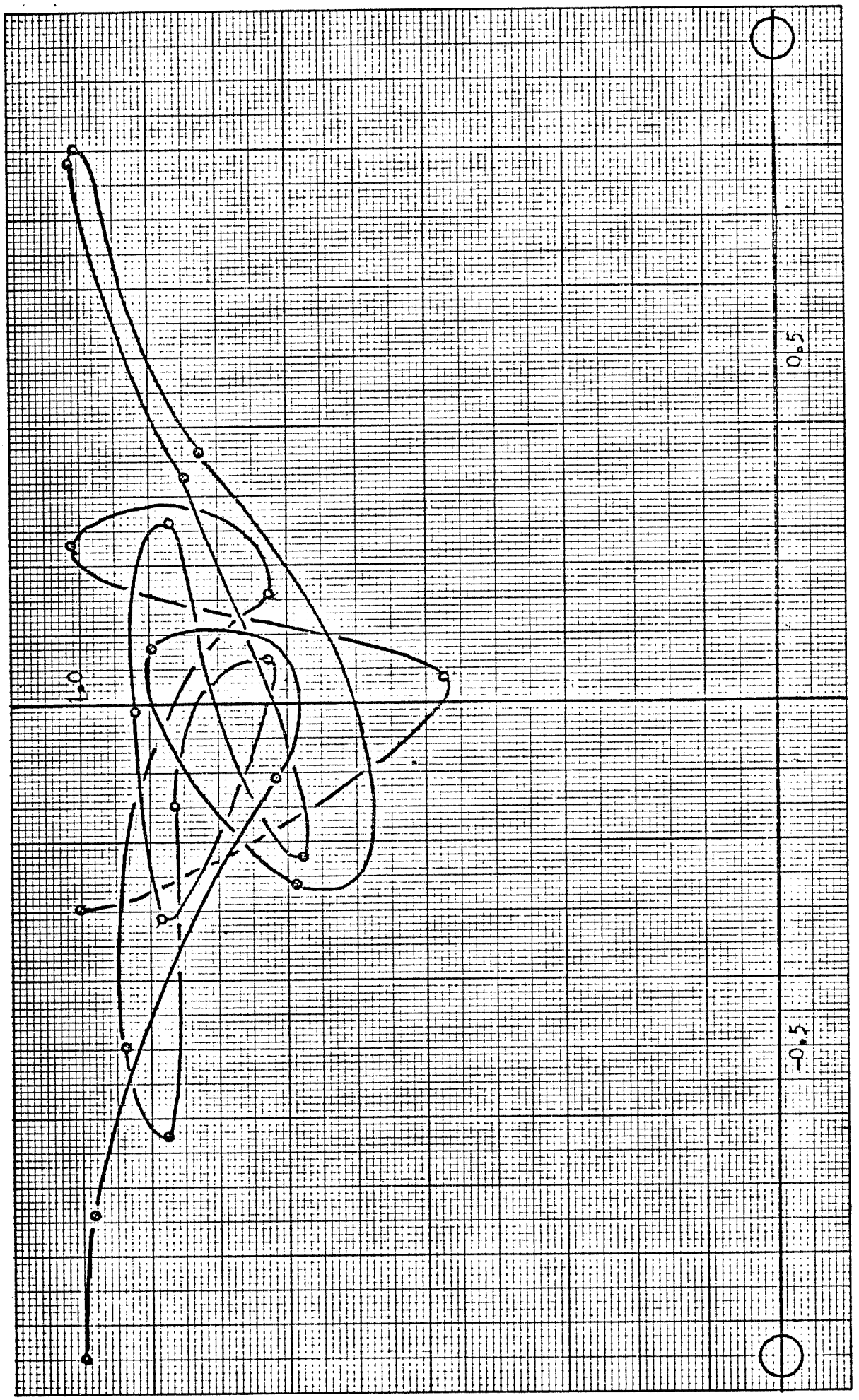


FIGURE 4(a)

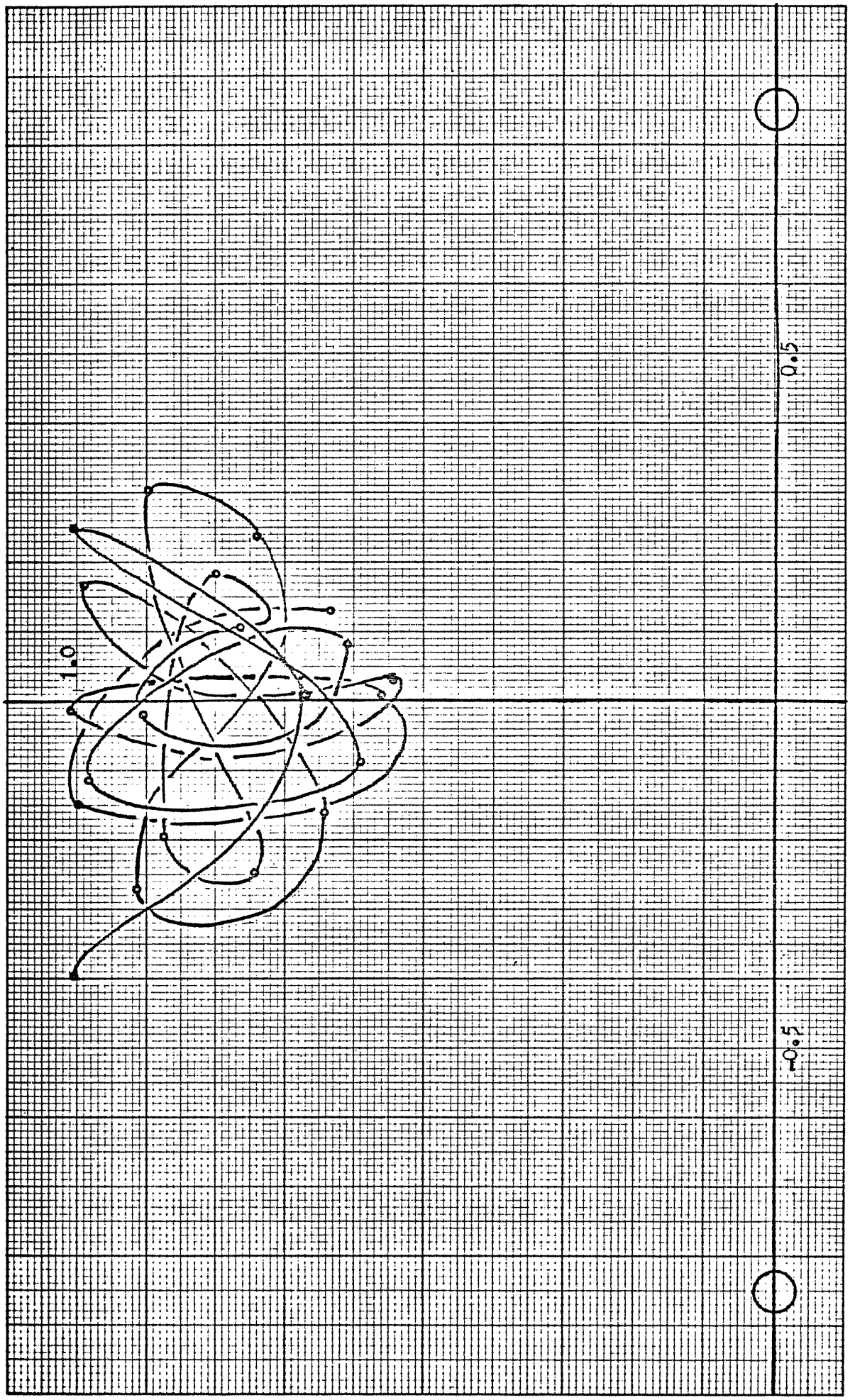


FIGURE 4(b)

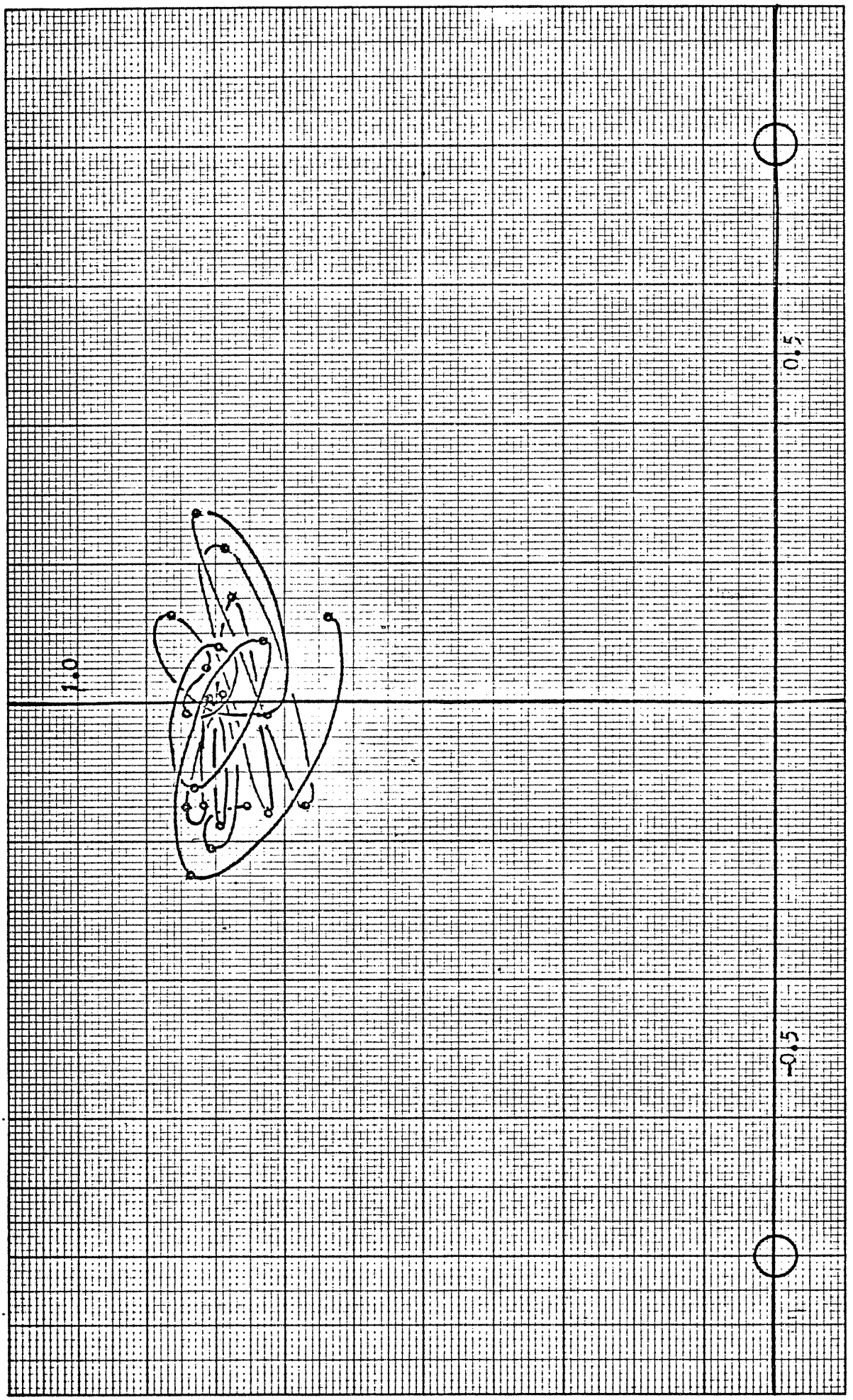


Figure 4(c)

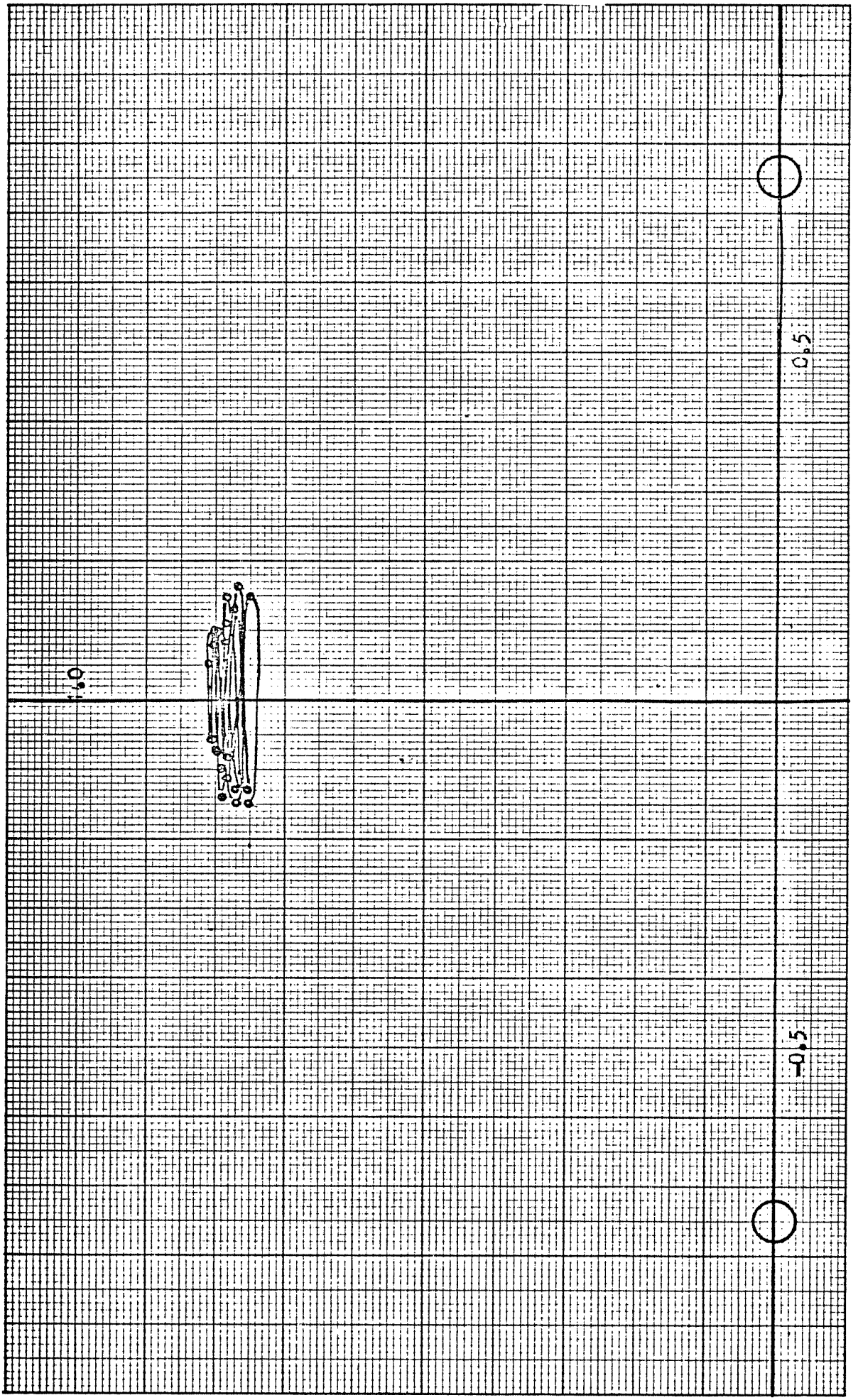


Figure 4(d)

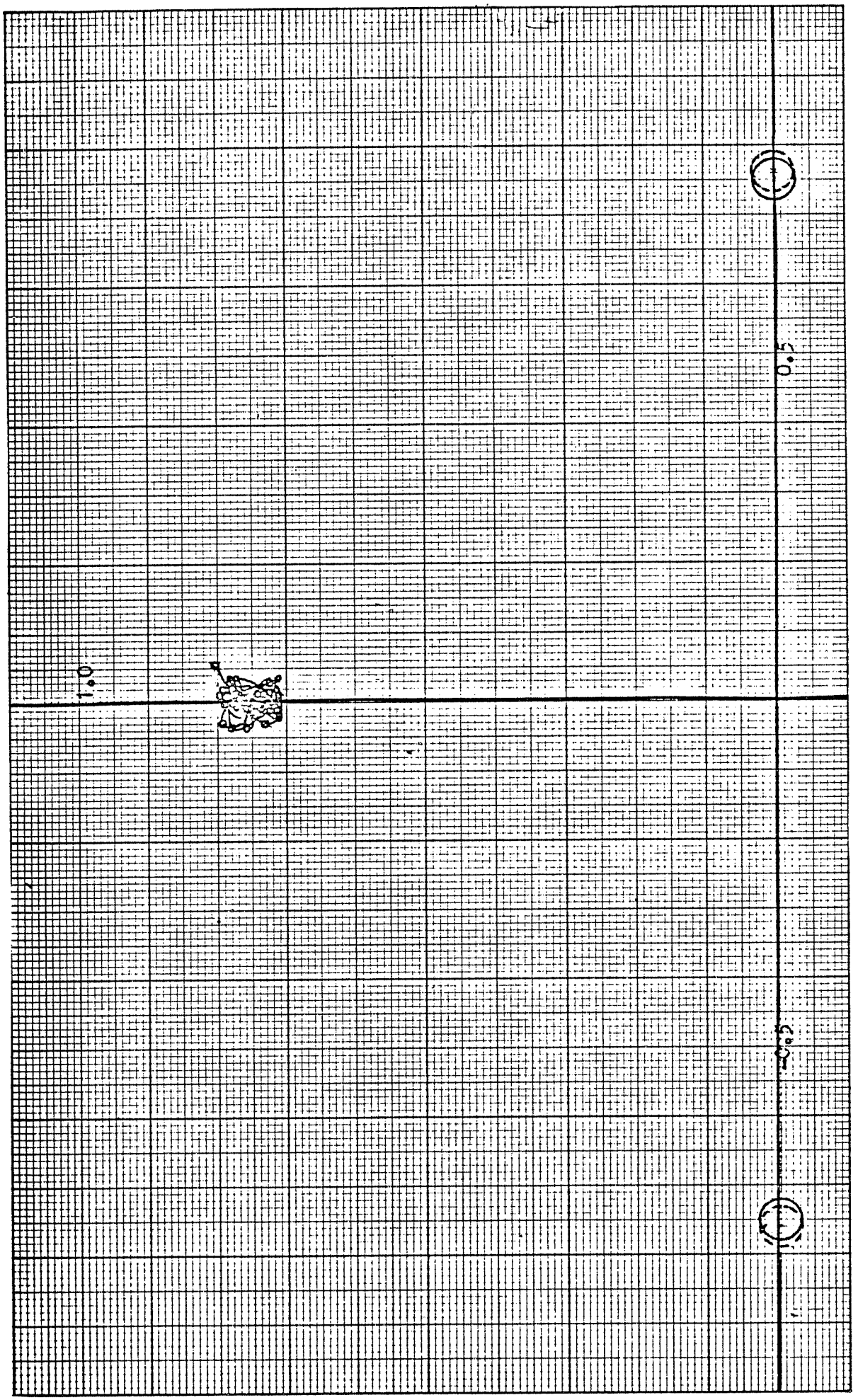


FIGURE 4(e)

6. A "Helium" Atom

In consideration next of an atom which has two protons, new forces must be considered. The exact nature of these forces depends on the particular nuclear model selected, the most popular of which are the liquid-drop, the optical, and the shell models [1,3,4,7,13-15,17]. However, no model yet developed yields a clear and unambiguous description of the forces within the nucleus [7]. For this reason, we will proceed in the following simplistic, qualitative way. Within the nucleus, assume that protons not only repel like $\frac{1}{r^2}$, but that they also attract like r^q , $q > -2$, with the net result being nuclear binding [7,15,17]. In particular, let P_1, P_2 be protons within a nucleus. Let P_3, P_4 be electrons. As in Section 5, let $m_1 = m_2 = 1600$, $m_3 = m_4 = 1$, $e_1 = e_2 = 40$, $e_3 = e_4 = -40$. Let the force $\vec{F}$ between any proton and any electron have magnitude F given by (4.2), that is by

$$F = -\frac{1600}{r^2} + \frac{1600}{r^9} \tag{6.1}$$

Let the force between the electrons have magnitude

$$F = \frac{1600}{r^2} \tag{6.2}$$

Finally, let the force between the nuclear protons have magnitude

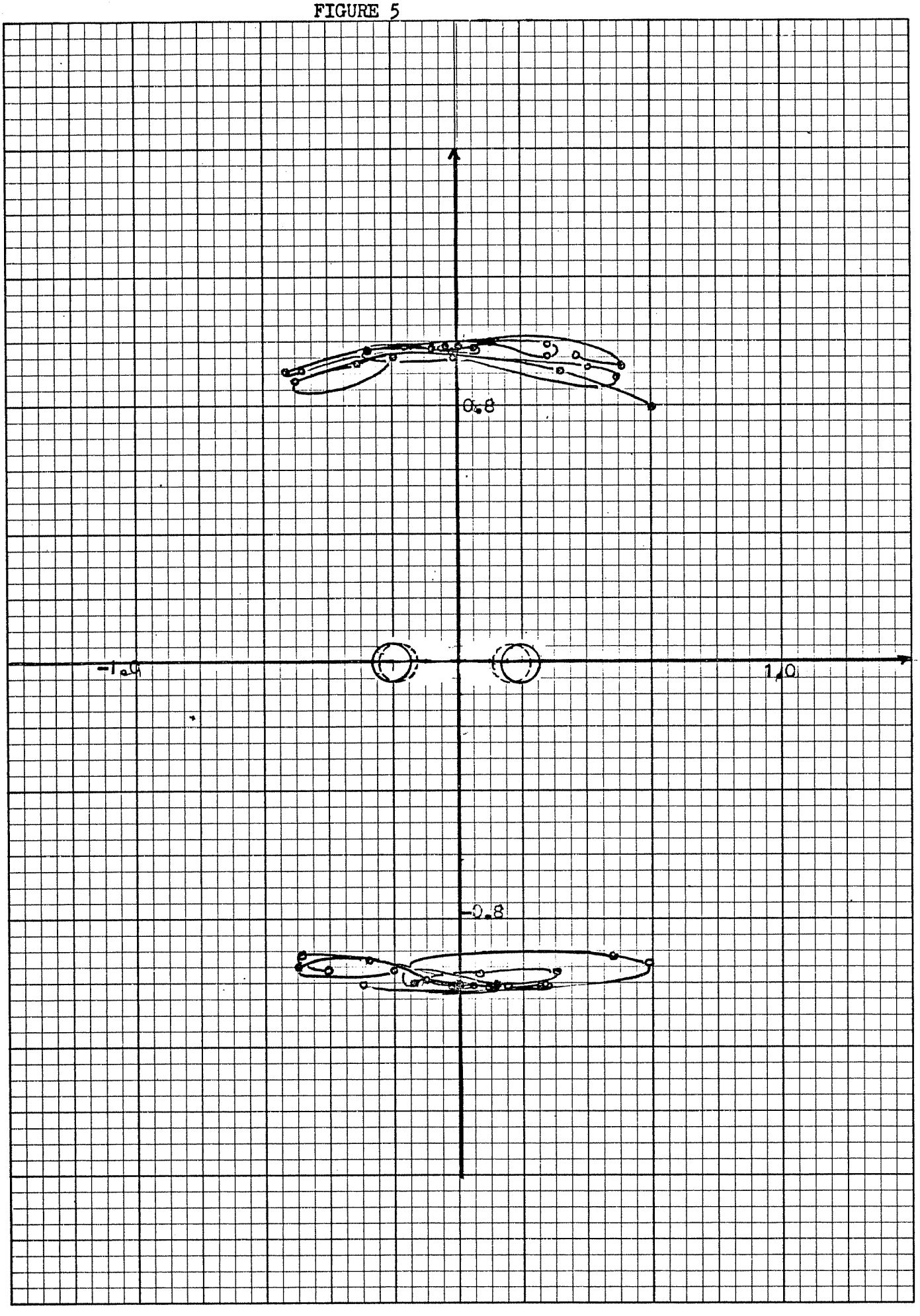
$$F = \frac{1600}{r^2} - 1600\, r^q \quad , \quad q > -2 \quad . \tag{6.3}$$

With this formulation, let us study stable configurations of this helium-like atom by varying the parameter q.

Suppose that the average distance between the protons is known, and, for illustrative purposes, let it be 0.4 . (Any other choice for this average distance could be treated in a fashion which is completely analogous to that which follows). Consider the initial data $x_{1,0} = 0.2$, $y_{1,0} = 0.0$, $x_{2,0} = -0.2$, $y_{2,0} = 0.0$, $x_{3,0} = 0$, $y_{3,0} = 1.0$, $x_{4,0} = 0$, $y_{4,0} = -1.0$, $\vec{v}_{i,0} \equiv 0$, $i = 1,2,3,4$. Then, for the choices $q = 3,5,6,7,9,12$, only the choice $q = 6$ resulted in each proton oscillating to both sides of its given initial position. Thus, for example, for $q = 3,5$, P_1 oscillated in such a fashion that $0 < x_{1,k} \leq 0.2$, for all k, while for $q = 7,9,12$, P_1 oscillated in such a fashion that $0.2 \leq x_{1,k}$ for all k. Thus, the choice $q = 6$ was selected as being physically reasonable for the particular proton configuration selected and the resulting proton and electron motions were completely stable, with each electron's maximum oscillation from its initial position being 0.0017 and each proton's maximum oscillation from its initial position being 0.0028.

To test the stability of the above atom, P_3 was reset to (0.6, 0.8) . Figure 5 then shows the electron and proton motions up to t_{10000}. The electron motion is given every 500 time steps. Though the proton motions are almost negligible, the second electron, by the time t_{6500} has begun a resonant vibration which thereafter continues with the motion of the first electron. The electrons, again, oscillate about a section of a circle which, this time, has a radius which is slightly smaller than the unit circle. Periodic graphing of electron positions is again consistent with the electron cloud concept of quantum mechanics, but in this particular example the motion is limited to that subsection of the cloud for which $-0.6 \leq x \leq 0.6$.

FIGURE 5



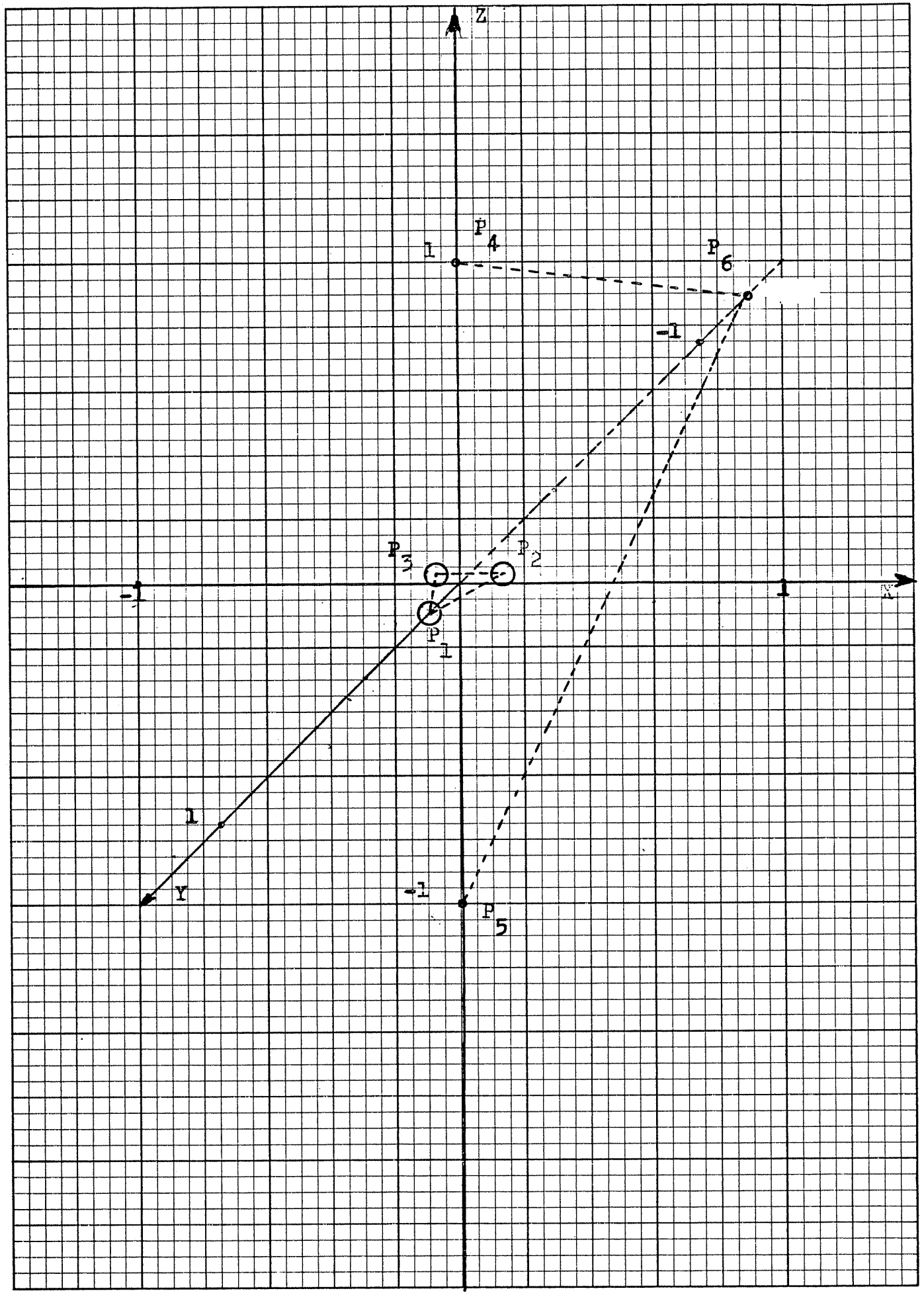
7. A "Lithium" Atom

Of necessity, we must now turn to three dimensions in order to consider an atom which consists of three electrons and three protons. We continue to avoid those complexities inherent in the existence of spin and of neutrons.

Let us describe first the intuition used in the choice of the initial data. Motivated by the results of Section 6 and desirous of producing greater proton motion than that described in Figure 5, we first set the three protons P_1, P_2, P_3 at the vertices of an equilateral triangle which lies in the XY plane, has side 0.2 units, and has the origin for its centroid. The vertices were taken at (0, 0.115, 0), (0.1, -0.058, 0), (-0.1, -0.058, 0), as shown in Figure 6. Next, the two electrons P_4 and P_5 were positioned at (0, 0, 1) and (0, 0, -1), which are symmetric with respect to the origin and should be relatively stable choices. Finally, in order to choose what is possibly a relatively stable position for electron P_6, we set it equidistant from electrons P_4 and P_5 and yet relatively close to the protons by choosing its initial position to be (0, -1.2, 0).

With these initial positions, as shown in Figure 6, and with $\vec{0}$ initial velocities, the system was allowed to interact for 200000 time steps. The particles all exhibited planar, oscillatory behavior which is shown every 500 time steps for the time period $t_{175,000}$ -t_{200000} in Figure 7 and is summarized as follows. For P_1, $x_{1,k} \equiv z_{1,k} \equiv 0$ while $0.12 \leq y_{1,k} \leq 0.31$. For P_2, $z_{2,k} \equiv 0$ while $0.10 \leq x_{2,k} \leq 0.27$ and $-0.15 \leq y_{2,k} \leq -0.06$. The results for P_3 are identical with those of P_2 except that $-0.27 \leq x_{3,k} \leq -0.10$. For P_4, $x_{4,k} \equiv 0$ while $-0.19 \leq y_{4,k} \leq 0.85$ and $066 \leq z_{4,k} \leq 1.04$. The results for P_5 are identical with those of P_4 except that $-1.04 \leq z_{5,k} \leq -0.66$. For P_6, $x_{6,k} \equiv z_{6,k} \equiv 0$ while $-1.28 \leq y_{6,k} \leq -0.98$. The centroid

FIGURE 6



of the system is, to two decimal places, always at the origin. The variation of the distances $r_{i,k}$ of P_i to the origin were $0.12 \leq r_{1,k} \leq 0.31$, $0.11 \leq r_{2,k} \leq 0.31$, $0.11 \leq r_{3,k} \leq 0.31$, $0.99 \leq r_{4,k} \leq 1.12$, $0.99 \leq r_{5,k} \leq 1.12$, $0.98 \leq r_{6,k} \leq 1.27$, with the average distances being $\bar{r}_{1,k} = 0.215$, $\bar{r}_{2,k} = 0.210$, $\bar{r}_{3,k} = 0.210$, $\bar{r}_{4,k} = 1.05$, $\bar{r}_{5,k} = 1.05$, $\bar{r}_{6,k} = 1.13$. Thus the third electron P_6 is, on the average a greater distance from the origin than are the two other electrons P_4 and P_5 . In quantum mechanical terms one would say that P_4 and P_5 are first level electrons while P_6 is a second level electron. Because of the relatively small numbers involved, it may be also that P_1 is a second level proton with respect to P_2 and P_3 , but this is clearly speculative only.

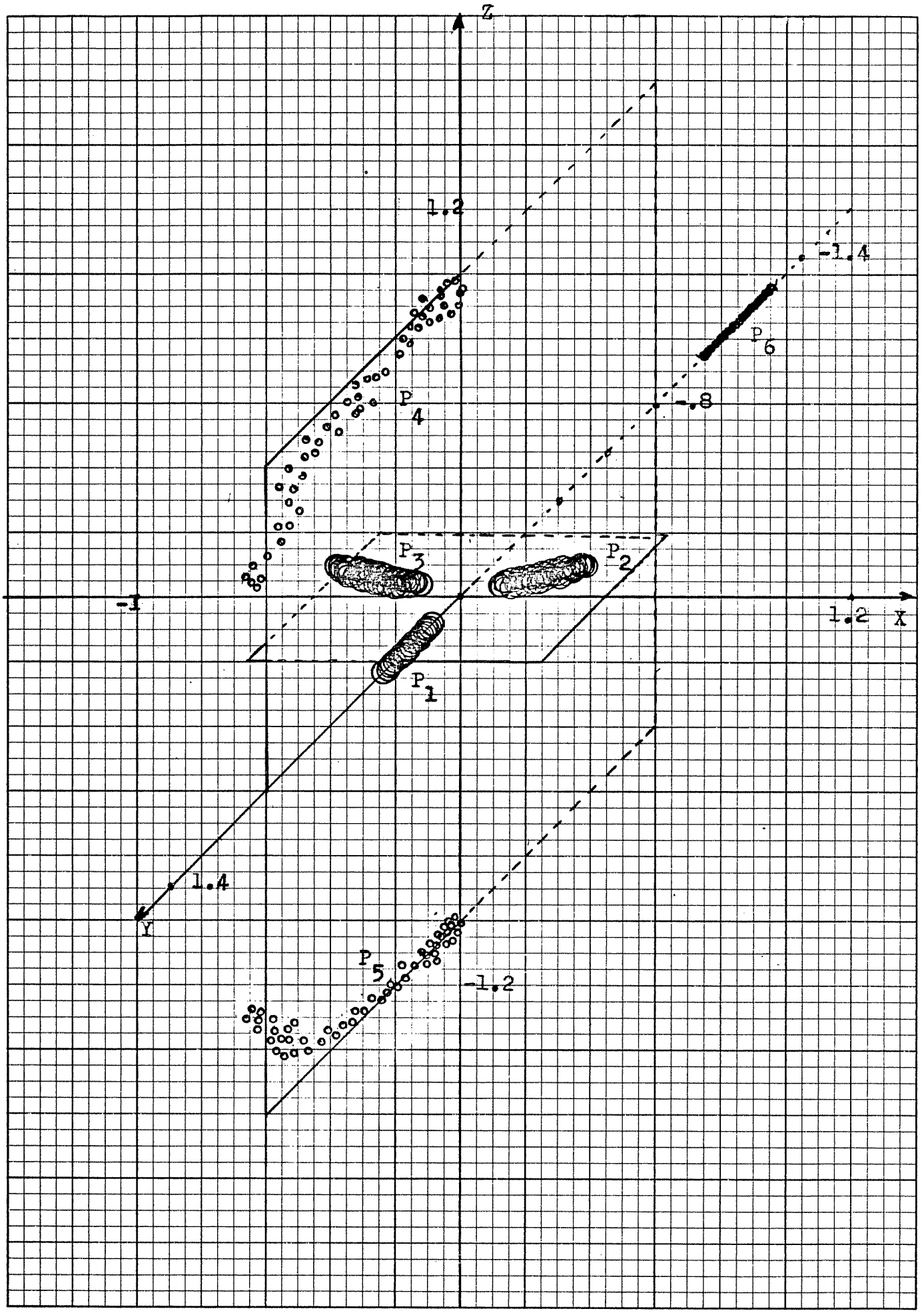
A variety of other calculations led to motions within "electron clouds" which were completely analogus to those described above. This was the case, for example, after resetting P_4 and P_5 at (0, 0.4, 0.92) and (0, 0.4, -0.92), respectively, and allowing interaction over 400,000 time steps. However, resetting P_6 too far from the origin, as was the case for the choice (0, -10.0, 0), resulted in P_6's approaching the origin with such a high speed that it was repelled with a force which eliminated it from all further effective interaction with the system.

8. Remarks

Further computations and modeling beyond that described already were not possible due to the termination of computing funds. In this section, then, let us discuss some of the many interesting questions which remain to be explored.

With regard to the computations already described, each should be repeated using real physical parameters, wherever these are available. Spin should be introduced wherever its existence has been established

FIGURE 7



experimentally. The presence of neutrons should be explored and, for example, one might examine on the computer possible reasons why ^{4}He is exceptionally stable why ^{5}He cannot be made to hold together [7].

With regard to calculations still to be done, computer experimentation with the beryllium atom would be most interesting because of the variety of possible electron, proton, and neutron initial configurations. Also, any eventual computer deduction of the correct bonding angle of the water molecule, i.e., 104.5° , would be superb. Finally, a computer explanation of the great emphasis which Pauling [16] places on the resonance mechanism in covalent bonding would be of wide interest.

Experimentally, with regard to the simplest atom, hydrogen, it would be of interest to explore the existence of energy states from a constructive, rather than a quantum mechanical descriptive, point of view. The existence of energy states with the well-known [15] electronic orbit radius formula

$$r = 0.5292n^2 \text{ A} \quad , \quad n = 1,2,... \tag{8.1}$$

should be examined in a most precise, experimental fashion, to determine whether or not the H-H energy curve has relative extrema or inflections at the values prescribed by (8.1) , contrary to the usual smooth curve energy representation.

Finally, it would be of interest to deduce the electron-structure configuration described by quantum mechanics by developing first a new and appropriate theory of nuclear structure. After all, the electrons are relatively free and of exceptionally light mass. They move rapidly and respond readily to the relatively massive, relatively tightly

bound nucleons. It seems plausible, then, that electron arrangement and motion should be deducible in a deterministic fashion from an appropriate theory of the nucleus, an idea which was hinted at in our model of the lithium type atom in Section 7.

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      IP1=I+1
      DO 76 J=IP1,N
      R2=(X(I,1)-X(J,1))**2+(Y(I,1)-Y(J,1))**2
      R=SQRT(R2)
C LONG RANGE FORCES ARE ELECTROSTATIC ATTRACTION OF UNLIKE CHARGES, R
C LIKE CHARGES, VARYING AS 1/R**2.  SHORT RANGE FORCES ARE REPULSIVE
C VARY WITH THE MASSES LIKE 1/R**P, THUS ALLOWING ELECTRONS TO
C MOVE EASILY, BUT NOT PROTONS.  SHORT RANGE REPULSION IS, HOWEVER, R
C TO ELECTRON-PROTON INTERACTIONS.
      IF (ABS(PMASS(I)-PMASS(J)).LT.0.1) GO TO 73
       F=(PCHARG(I)*PCHARG(J)/R**2)+(PMASS(I)*PMASS(J)/R**9)
      GO TO 74
73      F=PCHARG(I)*PCHARG(J)/R**2
74      FX=F*(X(I,1)-X(J,1))/R
      FY=F*(Y(I,1)-Y(J,1))/R
C ACCUMULATION OF FORCES ON PARTICLE I DUE TO ALL OTHER PARTICLES IS
C IN NEXT FOUR FORMULAS
75     ACX(I)=ACX(I)+FX
      ACX(J)=ACX(J)-FX
      ACY(I)=ACY(I)+FY
      ACY(J)=ACY(J)-FY
76     CONTINUE
77     CONTINUE
C NOTE THAT WE HAVE JUST ACCUMULATED FORCES, NOT ACCELERATIONS - THE
C NOTATION, THOUGH MISLEADING, ENABLES US TO SAVE MEMORY LOCATIONS.
C NEXT CALCULATE THE VELOCITIES AND POSITIONS AS FOLLOWS.
C ACTUAL ACCELERATIONS ARE INCLUDED BY DIVISION BY MASS OF 75 DIRECTL
C LEAP FROG FORMULAS ARE USED BUT SPECIAL STARTERS ARE NOT SHOWN BECA
C PROGRAM HERE CONTINUES CALCULATIONS FROM PUNCHED OUTPUT.
79     DO 799 I=1,N
      VX(I,2)=VX(I,1)+.0001*ACX(I)/PMASS(I)
      VY(I,2)=VY(I,1)+.0001*ACY(I)/PMASS(I)
      X(I,2)=X(I,1)+.0001*VX(I,2)
      Y(I,2)=Y(I,1)+.0001*VY(I,2)
799     CONTINUE
800     K=K+1
C PRINT ONLY EVERY KPRINT STEPS
      IF (MOD(K,KPRINT).GT.0) GO TO 82
      DO 810 I=1,N
      PRINT 81,K,I,X(I,2),Y(I,2),VX(I,2),VY(I,2)
81      FORMAT (5X,2I7,4F12.4)
810     CONTINUE
C TERMINATION AFTER A FIXED NUMBER OF STEPS
82      IF (K.LT.100000) GO TO 65
C PUNCH OUTPUT FOR RESTART
      PUNCH 10, (PMASS(I),PCHARG(I),X(I,2),Y(I,2),VX(I,2),VY(I,2),I=1,
      STOP
      END
```