

THE SUPERSYMMETRIC DIRAC EQUATION

The Application to Hydrogenic Atoms

Allen Hirshfeld



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Paul Dirac photograph by A. *Börtzells Tryckeri*, courtesy of AIP Emilio Segre Visual Archives, E. Scott Bar and Weber Collections.

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I wish to dedicate this book to the memory of my father, Dr. Martin A. Hirshfeld,
who taught me many things, among them the meaning of proof.

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Preface

One morning, when I was an undergraduate, over a cup of coffee in the cafeteria of the Weizman Institute, where he was working on his PhD in physics, Charles Robinson opened my eyes to the wonders of the Dirac equation, and sowed the seed for this book.

I met Paul Dirac in the early 1960s, on the occasion of his visit to the Physics Department of the Tel-Aviv University. We talked about my physics project at that time (I was working on my Master's thesis), and I attended his talk, where he explained the difficulties in the foundations of quantum field theory. Afterwards he autographed his book for me.

I am very grateful to Jens Peder Dahl, Professor Emeritus of the Chemistry Department of the Technical University of Denmark, for the fruitful and encouraging correspondence on his work.

I wish to thank Dirk Fischer for his assistance with the technical aspects of the preparation of the manuscript, and especially for his help in the preparation of the figures.

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Chapter 1

Introduction

“He succeeded in combining quantum mechanics and the theory of relativity, . . . and introduced the idea of an antiparticle. . . . Unfortunately, only the expert can appreciate Dirac’s awesome work. To this day, that work has not lost any of its splendor.”

Martinus Veltman, *Facts and Mysteries in Elementary Particle Physics*, World Scientific Publishing, Singapore, 2003.

The sentiment expressed in this quotation is certainly true. But let us pause to consider the phrase “only the expert can appreciate Dirac’s awesome work . . .”. We expect a student beginning to study quantum field theory to understand the working of relativistic quantum theory as it applies to free particles. The next interesting case, that of a particle in a Coulomb field, is given at best a somewhat cursory treatment in most texts. But it was precisely this problem that was the test of the new theory — could it explain the fine structure in the spectrum of hydrogen? The fact of this success and the detailed structure that it predicts were the hallmark of the theory for many years. It was the work devoted to testing this structure, with the highest possible precision, which revealed the need for the radiative corrections of quantum electrodynamics and provided us with the most accurate evaluation of the fine structure, which we possess to the present day, and one of the most impressive successes in all of physics.

It is thus highly desirable that the modern student of relativistic quantum mechanics should have an appreciation of this decisive episode in the physics of the twentieth century. The advances of the theory in recent years have led to certain simplifications with respect to Dirac’s time. In particular, the discovery that supersymmetry plays a central role in the structure of the theory of a particle in a Coulomb field means that while gaining a mastery of this topic, students are at the same time gaining experience that will be of importance in appreciating the questions with which their future work will be concerned, namely, does supersymmetry play a role in the structure of the universe? Even if this question is, contrary to expectation, answered in the negative, the knowledge of supersymmetry

is valuable because it allows a better understanding of many solvable problems in physics, and because of the role it plays in mathematics.

Thus, the purpose of the present book is to impart to the reader the necessary “expertise” for appreciating the application of the Dirac theory to the hydrogen atom. It will become clear that most of the concepts can be introduced in the more familiar, non-relativistic context in an elementary fashion. We will also become acquainted with a previous attempt to derive the formula for the fine structure of hydrogen, due to Sommerfeld. In this work, the *identical* formula for the energy levels of the hydrogen atom was obtained, 12 years *before* Dirac. This was before the Schrödinger wave equation for the non-relativistic hydrogen atom, and before the discovery of the spin of the electron! It is built on the Bohr model of the atom, but takes into account the relativistic motion of the electron. We shall see that it characterizes the orbits by their *eccentricity*, in a way that agrees with the Dirac theory.

We also take advantage, in our exposition, of the opportunity provided to relive the highlights of the history of physics. Kepler’s observation that Mars, in its motion around the Sun, follows an elliptical orbit, marks the beginning of physics as a quantitative science. In subsequent years, this system of two bodies interacting through the influence of a central force has served as a model of such disparate motions as the collision of galaxies and the orbits of electrons about the nuclei of atoms. It is the latter development that concerns us here.

For a particle moving in a central force field the angular momentum vector $\mathbf{L}$ is conserved. If the force is inversely proportional to the distance squared there is another conserved vector, the Laplace vector $\mathbf{A}$. The Laplace vector lies along the fixed axis of the orbital motion, and its magnitude is a measure of the eccentricity $e = |\mathbf{A}|$, which characterizes the deviation of the orbit from a circle. The Laplace vector turns out to be one of the central concepts of the book. The three components of the angular momentum, complemented by the three components of the Laplace vector, form, properly normalized, the generators of an $SO(4)$ symmetry group.

The Rutherford [Rut11] picture of the atom as a miniature solar system suggested an approach to understanding the spectral lines of light emitted in atomic transitions. With Bohr’s [Boh13] “quantum rules”, based on the postulate of a smallest unit of orbital angular momentum, the era of the “old quantum theory” was initiated.

A more refined version of the Bohr model is a non-relativistic form of Sommerfeld’s model [Som16], based on the Sommerfeld–Wilson quantization rules. The set of elliptical orbits predicted in the classical theory is reproduced, along with the formula for their eccentricity.

The beginning of the “new quantum theory” was marked, as a matter of fact, by Pauli’s [Pau26] group theoretical treatment of the hydrogen atom. Pauli’s analysis is based on the existence of the Laplace vector $\mathcal{A}$ as a conserved quantity of the motion of a point particle moving under the influence of an inverse-quadratic force. Its three components form, together with the three components of the orbital angular momentum, the generators of the Lie algebra $\mathfrak{so}(4)$. The quadratic Casimir operator of this algebra then yields a formula for the spectrum of the bound-state energy levels of hydrogenic atoms. The advantage of this approach over Schrödinger’s [Sch26] method of solving a differential equation is that it automatically yields an understanding of the degeneracy of the spectral lines, which is treated in the Schrödinger approach as an “accidental” symmetry.

A full analysis of the problem of an electron with spin in a Coulomb field involves the two-component Pauli formalism. It is only necessary to replace $\mathbf{p}$ by $(\boldsymbol{\sigma} \cdot \mathbf{p})$ to get the correct gyromagnetic ratio. The inclusion of the spin variables provides a formalism in which quadratic operators of the theory factorize. The effectiveness of such factorizations was already noted by Hull and Infeld [HI51], whose work was in a sense a precursor of the theory of supersymmetry, which arose originally in the quantum field theory of elementary particles. The Schrödinger equation for the radial component of the wave function is seen to be the product of two linear differential operators, whose eigenvalues are related to the magnitude of the operator $A_{nr} = (\boldsymbol{\sigma} \cdot \mathcal{A})$, in a way that is the quantum version of the eccentricity formula $e = |\mathcal{A}|$. Couching the results of the treatment of spin in a supersymmetric language leads to an understanding of the full degeneracy of the hydrogen spectrum as a consequence of the $\mathrm{SO}(4) \times \mathrm{S}(2)$ supersymmetry group.

When we ask for an understanding of the *fine structure* of the spectrum we move on to the treatment of the relativistic spectrum. Today we undertake a study of the solutions of the Dirac equation describing an electron in a Coulomb potential. In this book we first follow in the footsteps of Sommerfeld, who undertook a treatment of the relativistic problem, although he had at his disposal neither the modern quantum theory nor the notion of electron spin. It is all the more astonishing that he obtained a formula for the spectrum of hydrogen that agrees with the results of the Dirac theory. The Sommerfeld theory not only gives the correct formula for the energy of the hydrogen orbits, it also describes their relativistic eccentricity. One of the purposes of this book is to explain this success, based on the work of Biedenharn [Bie83].

When we go over to the relativistic problem the $\mathrm{SO}(4)$ symmetry breaks down, but a remnant of the Laplace vector survives, namely the Johnson–Lippmann operator A [JL50]. The Johnson–Lippmann operator is, in the non-relativistic

approximation, the operator A_{nr} . In this way the degeneracy of the spectrum reduces to that of $SO(3) \times S(2)$, with $SO(3)$ the symmetry generated by the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$, where $\mathbf{S}$ is the spin vector that generates the $SO(3)$ rotation group, and $S(2)$ is the supersymmetry group.

By describing the Dirac theory in a supersymmetric framework we are able to derive the solutions directly, without resorting to the heuristic methods employed formerly. Here we follow the work of Dahl and Jørgensen [DJ95]. The solutions of the Dirac equation are obtained by investigating two different extensions of the solution space. We describe the relation of the solutions to the second-order Kramer's equation, which was used formerly to construct solutions of the Dirac equation.

Finally, the non-relativistic approximations of the solutions found for the Dirac equation are shown to reduce to the solutions of the Pauli equation. This justifies the choice of sign for the solutions, and allows a check on the various normalization factors used in this book.

The Appendices deal with some of the features of the confluent hypergeometric functions, and their relation to the wave functions of the Pauli and Dirac equations.

The $SO(3) \times S(2)$ symmetry of the Dirac theory is broken by the radiative corrections of quantum field theory, notably in the Lamb shift [LR47], which describes the energy difference between the $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ levels of hydrogen. Because of this, the Dirac theory of bound states belongs in a course of study after non-relativistic quantum mechanics and before the introduction to the quantum theory of interacting fields. It is for such students that the present book is intended.

A note on units

This book uses the system of units in which $\hbar$ and the velocity of light are set to unity: $\hbar = c = 1$, where $\hbar = h/(2\pi)$, and h is Planck's constant. The Einstein convention is used throughout, according to which an index that appears in an expression twice is summed over. The fine structure constant is $\alpha = e^2/4\pi$, where e is the charge of the electron.

Chapter 2

The Classical Kepler Problem

“It is not eighteen months since I first caught a glimpse of the light, three months since the dawn, very few days since the unveiled Sun, most admirable to gaze upon, burst upon me. Nothing restrains me; I shall indulge my sacred fury; I shall triumph over mankind by the honest confession that I have stolen the golden vases of the Egyptians to build up a tabernacle for my God far from the confines of Egypt. If you forgive me, I rejoice; if you are angry, I can bear it; the die is cast, the book is written, to be read either now or by posterity, I care not which; it may well wait a century for a reader, as God himself has waited six thousand years for someone to behold his work.”

Johannes Kepler, *Gesammelte Werke*, 18 volumes, C. H. Beck, Munich, 1937–1969.

We are all familiar with the modern understanding of our solar system. The Sun sits at the center of a ring of essentially concentric orbits, each planet following an elliptical path around the Sun, which sits not at the center but at one focus of the ellipse. It is the picture shown in Figure 2.1. No one has ever seen this picture. Even today there are no satellites sitting at that vantage point tracking the orbits and plotting their paths, much less in the seventeenth century when this picture was first proposed by Johannes Kepler. Kepler and the astronomers before and since him have constructed their understanding of the solar system by watching the Sun and planets, observable as points of light, move across the sky. We only see this two-dimensional projection of their paths.

Kepler’s “unveiled Sun” was the realization that the observational data of Tycho Brahe, his mentor, could be explained by the following three laws:

- A planetary orbit is an ellipse with the Sun at one focus.
- A planetary orbit sweeps out equal areas in equal times.
- The square of the period of the orbit is directly proportional to the cube of its mean distance.

Kepler’s laws of motion were explained by Newton. Newton was able to show that they could be deduced from his universal law of gravitation, involving a central

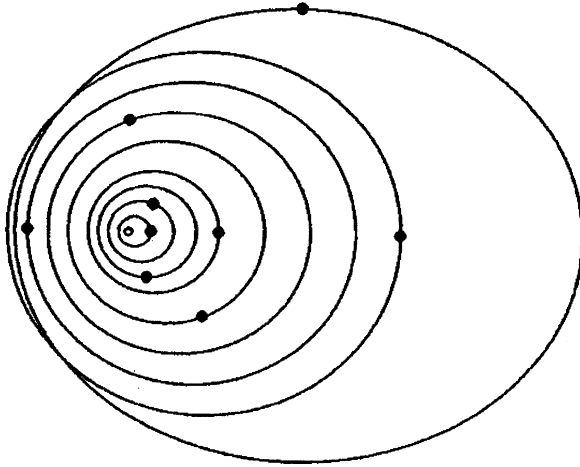


Figure 2.1. The solar system as we understand it.

force that falls off as the square of the distance. Taking the mass of the central attractor as infinite and the planet as a point particle leads to the problem of a point mass in a central potential field. The motion takes place in a fixed plane because of the conservation of angular momentum. The fact that the major axis of the ellipse remains stationary for a $1/r$ potential was known, by the time of Laplace, to be due to the conservation of the Laplace (Runge–Lenz) vector [Gol75], whose magnitude is equal to the eccentricity of the ellipse. With the model of an atom as a miniature solar system these concepts became relevant to the motion of electrons about the nucleus.

2.1 Central Forces

The velocity of the point P in space is

$$\mathbf{v} = \frac{d\mathbf{r}}{dt} = \frac{dr}{dt}\hat{\mathbf{r}} + r\frac{d\hat{\mathbf{r}}}{dt} = \frac{dr}{dt}\hat{\mathbf{r}} + r\frac{d\theta}{dt}\hat{\boldsymbol{\theta}}, \quad (2.1)$$

where $\mathbf{r} = r\hat{\mathbf{r}}$ is the position vector and $\hat{\mathbf{r}}$ is a unit vector on the direction of $\mathbf{r}$. $\hat{\boldsymbol{\theta}}$ is a unit vector perpendicular to $\hat{\mathbf{r}}$:

$$\hat{\mathbf{r}} = (\cos \theta(t), \sin \theta(t)), \quad \hat{\boldsymbol{\theta}} = (-\sin \theta(t), \cos \theta(t)). \quad (2.2)$$

The acceleration is

$$\begin{aligned}\mathbf{a} &= \frac{d\mathbf{v}}{dt} = \frac{d^2r}{dt^2}\hat{\mathbf{r}} + 2\frac{dr}{dt}\frac{d\theta}{dt}\hat{\boldsymbol{\theta}} + r\frac{d^2\theta}{dt^2}\hat{\boldsymbol{\theta}} + r\frac{d\theta}{dt}\left(-\frac{d\theta}{dt}\hat{\mathbf{r}}\right) \\ &= \left(\frac{d^2r}{dt^2} - r\left(\frac{d\theta}{dt}\right)^2\right)\hat{\mathbf{r}} + \frac{1}{r}\frac{d}{dt}\left(r^2\frac{d\theta}{dt}\right)\hat{\boldsymbol{\theta}}.\end{aligned}\quad (2.3)$$

Equation (2.3) tells us that the acceleration is entirely radial, that is, parallel to $\mathbf{r}$, if and only if

$$\frac{d}{dt}\left(r^2\frac{d\theta}{dt}\right) = 0, \quad (2.4)$$

which is equivalent to saying that $r(t)^2 d\theta/dt$ is a constant independent of t .

Combining this with the next lemma gives a proof of Kepler's second law:

Lemma. If the position of a particle over time is described by the vector function $\mathbf{r}(t)$, then the rate at which the radial vector sweeps out area is given by

$$\frac{dA}{dt} = \frac{r(t)^2}{2} \frac{d\theta}{dt}. \quad (2.5)$$

Proof. Given a circle with center at the origin and radius r , the area swept out by the radius as it moves through an angle of $\Delta\theta$ is given by $(r^2/2)\Delta\theta$. It follows that if ΔA is the area swept out by the radial vector from time s to time t , and if the distance from the origin stays constant during this time interval, then

$$\Delta A = \frac{r^2}{2} \Delta\theta, \quad (2.6)$$

where $\Delta\theta = \theta(t) - \theta(s)$. If r does not stay constant, then we can find two points in the interval $[s, t]$, call them t_1 and t_2 , where r takes on its minimum and maximum values, respectively, over this interval: $r(t_1) \leq r \leq r(t_2)$. It follows that

$$\frac{r(t_1)^2}{2} \Delta\theta \leq \Delta A \leq \frac{r(t_2)^2}{2} \Delta\theta. \quad (2.7)$$

We now divide by $\Delta t = t - s$:

$$\frac{r(t_1)^2}{2} \frac{\Delta\theta}{\Delta t} \leq \frac{\Delta A}{\Delta t} \leq \frac{r(t_2)^2}{2} \frac{\Delta\theta}{\Delta t}, \quad (2.8)$$

and take the limit as s approaches t . This forces t_1 and t_2 to also approach t and yields

$$\frac{r(t)^2}{2} \frac{d\theta}{dt} \leq \frac{dA}{dt} \leq \frac{r(t)^2}{2} \frac{d\theta}{dt}. \quad (2.9)$$

Lemma. Let $\mathbf{r}(t)$ be the position of a particle at time t , and $\mathbf{v}(t)$ its velocity. The momentum of the particle is $\mathbf{p} = m\mathbf{v}$, where m is its mass. If the particle is moving under the influence of a central force:

$$\mathbf{F} = \frac{d\mathbf{p}}{dt} = f(r)\hat{\mathbf{r}}, \quad (2.10)$$

where f is an arbitrary function of r , then the orbital angular momentum

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \quad (2.11)$$

is a constant vector of magnitude

$$L = |\mathbf{L}| = mr(t)^2 \frac{d\theta}{dt}. \quad (2.12)$$

Proof. The fact that $\mathbf{L}$ is a constant vector is immediate:

$$\frac{d\mathbf{L}}{dt} = \frac{d}{dt}(\mathbf{r} \times \mathbf{p}) = m\mathbf{v} \times \mathbf{v} + f(r)\mathbf{r} \times \hat{\mathbf{r}} = \mathbf{0}. \quad (2.13)$$

To prove Eq. (2.12) we write

$$\mathbf{L} = mr\hat{\mathbf{r}} \times \left(\frac{dr}{dt}\hat{\mathbf{r}} + r\frac{d\theta}{dt}\hat{\boldsymbol{\theta}} \right) = mr^2 \frac{d\theta}{dt}(\hat{\mathbf{r}} \times \hat{\boldsymbol{\theta}}), \quad (2.14)$$

so that

$$L = mr^2 \frac{d\theta}{dt}. \quad (2.15)$$

Since

$$\mathbf{L} \cdot \mathbf{r} = (\mathbf{r} \times \mathbf{p}) \cdot \mathbf{r} = (\mathbf{r} \times \mathbf{r}) \cdot \mathbf{p} = 0, \quad (2.16)$$

the motion is in a plane perpendicular to $\mathbf{L}$.

2.2 The Laplace Vector

We now consider the case of a force inversely proportional to the square of the distance from the origin:

$$\mathbf{F} = \frac{d\mathbf{p}}{dt} = -\left(\frac{k}{r^2}\right)\hat{\mathbf{r}}. \quad (2.17)$$

Kepler's first law is a consequence of the following theorem:

Theorem. Let $\mathbf{r}(t)$ denote the position of a particle moving under the influence of a force inversely proportional to the square of the distance from the origin. Then

there exists a constant vector $\mathcal{A}$, the Laplace vector, such that

$$|\mathbf{r}| + \mathbf{r} \cdot \mathcal{A} = \frac{L^2}{mk}. \quad (2.18)$$

Equivalently, if (r, θ) is the position in polar coordinates, then

$$r(1 + e \cos \theta) = \frac{L^2}{mk}, \quad (2.19)$$

where the eccentricity e is equal to the magnitude of $\mathcal{A}$: $e = |\mathcal{A}|$. We recognize Eq. (2.19) as the equation of a conic section: an ellipse, parabola, or hyperbola. In particular, if $e < 1$, then it is the equation of an ellipse with one focus at the origin.

Proof. We note

$$L^2 = \mathbf{L} \cdot (\mathbf{r} \times \mathbf{p}) = (\mathbf{p} \times \mathbf{L}) \cdot \mathbf{r}. \quad (2.20)$$

Now

$$\begin{aligned} \frac{d}{dt}(\mathbf{p} \times \mathbf{L}) &= \frac{d\mathbf{p}}{dt} \times \mathbf{L} = \left(-\frac{k}{r^2} \hat{\mathbf{r}}\right) \times \left(mr^2 \frac{d\theta}{dt} \hat{\mathbf{r}} \times \hat{\boldsymbol{\theta}}\right) \\ &= -mk \frac{d\theta}{dt} [\hat{\mathbf{r}} \times (\hat{\mathbf{r}} \times \hat{\boldsymbol{\theta}})] = mk \frac{d\theta}{dt} \hat{\boldsymbol{\theta}} = \frac{d}{dt}(mk\hat{\mathbf{r}}). \end{aligned} \quad (2.21)$$

This means that the time derivative of $\mathbf{p} \times \mathbf{L} - mk\hat{\mathbf{r}}$ is zero, so

$$\mathcal{A} = \frac{1}{mk}(\mathbf{p} \times \mathbf{L}) - \hat{\mathbf{r}} \quad (2.22)$$

is a constant vector, and

$$\mathbf{p} \times \mathbf{L} = mk(\hat{\mathbf{r}} + \mathcal{A}). \quad (2.23)$$

Combining this result with Eq. (2.20), we see that

$$L^2 = (\mathbf{p} \times \mathbf{L}) \cdot \mathbf{r} = mk(|\mathbf{r}| + \mathbf{r} \cdot \mathcal{A}), \quad (2.24)$$

or

$$|\mathbf{r}| + \mathbf{r} \cdot \mathcal{A} = \frac{L^2}{mk}. \quad (2.25)$$

Equation (2.19) follows from the equalities $|\mathbf{r}| = r$ and $\mathbf{r} \cdot \mathcal{A} = re \cos \theta$.

An ellipse with foci F_1 and F_2 can be defined as the locus of points P for which $|F_1P| + |F_2P| = 2a$, with a the semimajor axis. The point P is described by the vector function $\mathbf{r}(t) = r(t)\hat{\mathbf{r}}(t)$, with $r(t) = \sqrt{x(t)^2 + y(t)^2}$ and $\hat{\mathbf{r}}(t) = (\cos \theta(t), \sin \theta(t))$. See Figure 2.2.

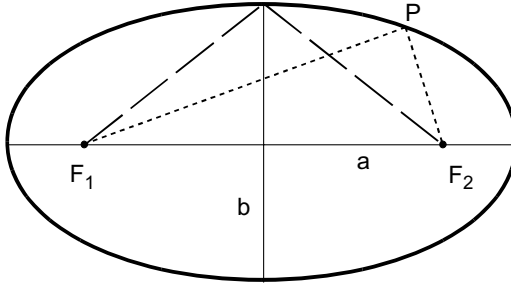


Figure 2.2. An ellipse.

Lemma. The general equation of an ellipse with one focus at the origin and semimajor axis along the x-axis is given in polar coordinates by

$$r(1 + e \cos \theta) = c, \quad (2.26)$$

where e and c are constants, $0 < e < 1$, $c > 0$. The semimajor axis is

$$a = \frac{c}{1 - e^2}, \quad (2.27)$$

and the semiminor axis is

$$b = \frac{c}{\sqrt{1 - e^2}}. \quad (2.28)$$

The *eccentricity* of the ellipse is

$$e = \sqrt{1 - (b/a)^2}. \quad (2.29)$$

Proof. Equation (2.26) can be rewritten as

$$r = c - er \cos \theta. \quad (2.30)$$

We convert this to Cartesian coordinates ($x = r \cos \theta$, $y = r \sin \theta$) and square each side to obtain

$$x^2 + y^2 = c^2 - 2ecx + e^2x^2, \quad (2.31)$$

or

$$(1 - e^2)x^2 + 2ecx + y^2 = c^2. \quad (2.32)$$

Now add $c^2e^2/(1 - e^2)$ to each side:

$$(1 - e^2)x^2 + 2ecx + \frac{c^2e^2}{1 - e^2} + y^2 = c^2 + \frac{c^2e^2}{1 - e^2}, \quad (2.33)$$



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or

$$(1 - e^2)(x + ea)^2 + y^2 = \frac{c^2}{1 - e^2}, \quad (2.34)$$

which may be rewritten as

$$\frac{(x + ea)^2}{a^2} + \frac{y^2}{b^2} = 1. \quad (2.35)$$

This is the equation of an ellipse in Cartesian coordinates. The center of the ellipse is at $(-ae, 0)$, which is a distance ae from the origin. The foci are bisected by a line that intersects the ellipse at two points. At these points the distance from the foci is $\sqrt{(ae)^2 + b^2} = a$, and the sum of the distances from the foci, which is the same for all points of the ellipse, is $2a$.

The *perigee*, which is the point of closest approach, corresponds to $\theta = 0$, so

$$r_{\min} = a(1 - e) = \frac{L^2}{mk(1 + e)}. \quad (2.36)$$

The *apogee*, which is the farthest distance, corresponds to $\theta = \pi$, so

$$r_{\max} = a(1 + e) = \frac{L^2}{mk(1 - e)}. \quad (2.37)$$

The *mean distance* is $\frac{1}{2}(r_{\min} + r_{\max}) = a$.

The Laplace vector $\mathcal{A}$ is perpendicular to the angular momentum,

$$\mathcal{A} \cdot \mathbf{L} = 0, \quad (2.38)$$

so $\mathcal{A}$ lies in the plane of motion of $\mathbf{r}$. As a matter of fact, $\mathcal{A}$ lies along the line joining the two foci.

We express the eccentricity in terms of the constants of the motion, the energy E , and the angular momentum L . We use the identities

$$\begin{aligned} (a) \quad (\mathbf{p} \times \mathbf{L}) \cdot (\mathbf{p} \times \mathbf{L}) &= p^2 L^2, \\ (b) \quad (\mathbf{p} \times \mathbf{L}) \cdot \mathbf{r} &= \mathbf{L} \cdot (\mathbf{r} \times \mathbf{p}) = L^2. \end{aligned} \quad (2.39)$$

We then have

$$|\mathcal{A}|^2 = \frac{p^2 L^2}{m^2 k^2} - \frac{2L^2}{mk r} + 1 = \frac{2L^2}{mk^2} \left(\frac{p^2}{2m} - \frac{k}{r} \right) + 1 = \frac{2L^2 E}{mk^2} + 1 = e^2, \quad (2.40)$$

where

$$E = \frac{p^2}{2m} - \frac{k}{r} \quad (2.41)$$

is the constant energy of a particle in a fixed orbit.

From the equation for the perigee we have

$$r_{\min} = a(1 - e) = \frac{L^2}{mk(1 + e)}, \quad (2.42)$$

or

$$1 - e^2 = \frac{L^2}{mka}. \quad (2.43)$$

Comparing this to Eq. (2.40):

$$1 - e^2 = -\frac{2L^2 E}{mk^2}, \quad (2.44)$$

we get

$$E = -\frac{k}{2a}. \quad (2.45)$$

The energy of a particle in orbit depends only on the semimajor axis of the ellipse.

We can now derive Kepler's third law. By Kepler's first law a particle in orbit moves on an ellipse. The semiminor axis of the ellipse is $b = a\sqrt{1 - e^2}$. By Kepler's second law the area of the ellipse is

$$A = \int_0^\tau \frac{dA}{dt} dt = \frac{L}{2m} \tau, \quad (2.46)$$

where τ is the period of a complete revolution. Hence

$$A = \frac{L}{2m} \tau = \pi ab = \pi a^2 \sqrt{1 - e^2} = \pi a^2 \frac{L}{k} \sqrt{\frac{-2E}{m}} = \pi a^{3/2} \frac{L}{\sqrt{km}}, \quad (2.47)$$

or

$$\tau = 2\pi a^{3/2} \sqrt{\frac{m}{k}}. \quad (2.48)$$

The square of the period of the orbit is therefore proportional to the cube of a , which is the mean distance.

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## Notes on Chapter 2

The conservation of the Laplace vector and the interpretation of its length as eccentricity are first mentioned by Jacob Hermann, in a letter to Bernoulli. It was then used by Laplace in his treatise on mechanics. It was rediscovered by Hamilton in the nineteenth century, and included in textbooks by Gibbs and Runge. Pauli learned about it from his teacher Lenz, and after Pauli's quantum mechanical treatment of the hydrogen atom (Chapter 8) it is commonly referred to as the Runge–Lenz vector. The early history of the Laplace vector was traced by Goldstein [Gol75] [Gol76]. See also the Wikipedia page at [http://en.wikipedia.org/wiki/Laplace–Runge–Lenz\\_vector](http://en.wikipedia.org/wiki/Laplace–Runge–Lenz_vector). The presentation here follows Bressoud [Bre91]. The origin of the Laplace vector as the boost-generator of the relativistic extension of the theory has been proposed by Dahl [Dah95].

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## Chapter 3

### Symmetry of the Classical Problem

*“Symmetry, as wide or as narrow as you may wish to define it, is one idea by which man through the ages has tried to comprehend and create order, beauty, and perfection.”*

Hermann Weyl, in *Symmetry*, Princeton University Press, Princeton, 1952.

In this chapter we make an excursion into mathematics. We first review the definitions of Lie groups and Lie algebras, because these are the mathematical basis of symmetry considerations in physics. We show how these concepts fit into the Hamiltonian formulation of classical mechanics. We then return to the problem of a central force which is inversely proportional to the square of the distance, and show that the conservation of the Laplace vector, together with the conservation of angular momentum, is equivalent to the existence of an  $SO(4)$  symmetry group that acts on functions of the phase space.

#### 3.1 Lie Groups and Lie Algebras

Let  $A$  be a linear operator on a finite dimensional vector space  $V$ . If  $V = \mathbb{R}^n$  then  $A$  is an  $n \times n$  matrix. The operator valued function  $t \mapsto e^{tA}$  is defined by

$$e^{tA} = I + tA + \frac{1}{2}t^2 A^2 + \frac{1}{3!}t^3 A^3 + \dots \quad (3.1)$$

which converges for all  $t$ . For a fixed  $A$ , the function  $e^{tA}$  behaves like the ordinary exponential function:

$$e^{tA}|_{t=0} = I, \quad e^{(t+s)A} = e^{tA}e^{sA}, \quad \frac{d}{dt}e^{tA} = Ae^{tA}. \quad (3.2)$$

$e^{tA}$  is a curve of linear operators, and the LHS of the last equation gives the tangent vector to this curve at time  $t$ . At  $t = 0$  we have

$$\frac{d}{dt}e^{tA}|_{t=0} = A.$$

If  $R$  is some other invertible operator then

$$(RAR^{-1})^n = RA^n R^{-1} \quad (3.4)$$

for all  $n$ , so

$$e^{t(RAR^{-1})} = Re^{tA}R^{-1}. \quad (3.5)$$

In particular, the tangent vector to  $Re^{tA}R^{-1}$ , which goes through the identity  $I$  at  $t = 0$ , is  $RAR^{-1}$ .

Suppose  $A$  is fixed and  $R(s)$  is a curve of matrices that passes through  $I$  at  $s = 0$  and is differentiable in  $s$ . Then  $R(s)$  is invertible for  $s$  close to the identity, and differentiating

$$R(s)R(s)^{-1} = I \quad (3.6)$$

at  $s = 0$  gives

$$\frac{d}{ds}R^{-1}(s)|_{s=0} = -\frac{d}{ds}R(s)|_{s=0} = -B, \quad (3.7)$$

and

$$\frac{d}{ds}[R(s)AR(s)^{-1}]_{s=0} = BA - AB, \quad (3.8)$$

by Leibniz's rule. Define the *Lie bracket*  $[ , ]$  by

$$[B, A] = BA - AB. \quad (3.9)$$

The Lie bracket is bilinear, antisymmetric, and satisfies Jacobi's identity:

$$\begin{aligned} [A, [B, C]] &= [A, BC - CB] = [A, BC] - [A, CB] \\ &= [A, B]C + B[A, C] - [A, C]B - C[A, B] \\ &= (AB - BA)C + B(AC - CA) \\ &\quad - (AC - CA)B - C(AB - BA) \\ &= [[A, B], C] + [B, [A, C]]. \end{aligned} \quad (3.10)$$

A subgroup  $G$  of the group of all invertible matrices is said to be a linear *Lie group* if it is also a closed manifold.

For example, let  $O(n)$  be the  $n \times n$  matrices that satisfy  $OO^T = I$ , where  $O^T$  denotes the transposed matrix. This defines  $O(n)$  as a subgroup of the  $n^2$  dimensional space of  $(n \times n)$ -matrices. Let  $R(s)$  be a curve of orthogonal matrices.

with  $R(0) = I$  and  $R'(0) = B$ . Differentiate  $R(s)R(s)^T = I$  at  $s = 0$ , and obtain

$$B + B^T = 0, \quad (3.11)$$

so  $B$  is antisymmetric. The dimension of the tangent space, and hence the manifold  $O(n)$ , is thus  $n(n-1)/2$ .  $O(3)$  is a three-dimensional subgroup of the nine-dimensional group of all invertible  $3 \times 3$  matrices.  $O(4)$  is six-dimensional.

Conversely, let  $A$  be an antisymmetric matrix.

$$(e^{tA})^T = e^{tA^T}, \quad (3.12)$$

since  $(A^T)^n = (A^n)^T$ .

$$\frac{d}{dt} [e^{tA}(e^{tA})^T] = \frac{d}{dt} [e^{tA}e^{tA^T}] = e^{tA}(A + A^T)e^{tA^T}. \quad (3.13)$$

But  $A + A^T = 0$ . Hence

$$\frac{d}{dt} [e^{tA}(e^{tA})^T] = 0. \quad (3.14)$$

At  $t = 0$ ,  $e^{tA}(e^{tA})^T|_{t=0} = I$ , hence for all  $t$

$$e^{tA}(e^{tA})^T = I. \quad (3.15)$$

If  $A$  is antisymmetric,  $e^{tA}$  is orthogonal.

Let  $G$  denote the Lie group  $O(n)$  and  $\mathcal{G}$  the space of antisymmetric matrices. Then  $\mathcal{G}$  is the tangent space of  $G$  at the identity. So if  $R(s)$  is a differentiable curve of matrices in  $G$  and  $R(0) = I$ , then  $R'(0) \in \mathcal{G}$ .

If  $A \in \mathcal{G}$  then the curve  $e^{tA}$  is a *one-parameter subgroup* of  $G$ .

The *Lie bracket* of two antisymmetric matrices is antisymmetric:

$$\begin{aligned} [A, B]^T &= (AB - BA)^T = B^T A^T - A^T B^T \\ &= [B^T, A^T] = -[A^T, B^T] = -[A, B]. \end{aligned} \quad (3.16)$$

But it is more instructive to derive this from the statements above. Indeed, let  $B \in \mathcal{G}$ . Then  $R(s) = e^{sB}$  is a curve of matrices in  $G$ . Hence for each fixed  $s$ , conjugation by  $R(s)$  carries  $G$  into itself, and carries  $I$  into itself, and hence must carry the tangent space  $\mathcal{G}$  into itself. Hence if  $A \in \mathcal{G}$ , the curve  $C(s) = R(s)AR(s)^{-1}$  lies in  $G$ ;  $C(s) \in G$  for all  $s$ . But then  $C(s+h) - C(s) \in G$  for any  $s$  and  $h$ . Dividing by  $h$  and passing to the limit implies  $C'(s) \in \mathcal{G}$ . At  $s = 0$  this tells us that for  $B \in \mathcal{G}$  and  $A \in \mathcal{G}$  also  $[B, A] \in \mathcal{G}$ .

The corresponding facts are true in general: If  $G$  is a linear Lie group then its tangent space  $\mathcal{G}$  at  $I$  is the space spanned by  $A \in \mathcal{G}$ , and the curve  $e^{tA}$  is a one-parameter subgroup of  $G$ . We say that  $\mathcal{G}$  is the *Lie subalgebra* of the space of all matrices.

More generally, a linear space  $\mathcal{G}$  with a bracket mapping  $\mathcal{G} \times \mathcal{G} \mapsto \mathcal{G}$  is called a *Lie algebra* if the bracket is bilinear, antisymmetric, and satisfies the Jacobi identity. A group  $G$  that is a finite-dimensional manifold, where the group multiplication is consistent with the manifold structure in an obvious way, is called a *Lie group*. The tangent space to  $G$  at  $I$  (in the sense of differentiable manifolds) then inherits the structure of a Lie algebra. Given any finite-dimensional Lie algebra  $\mathcal{G}$  over the real numbers, there always exists a Lie group  $G$  having  $\mathcal{G}$  as its Lie algebra. All such  $G$  will be “locally isomorphic”, but may differ in their global structure. There is a unique  $G$  that is connected and simply connected having  $\mathcal{G}$  as its Lie algebra.

### 3.2 Some Special Lie Algebras

We now discuss in more detail the Lie algebras with which we shall be concerned.

#### $\mathfrak{o}(3)$

Let  $\delta_i$  denote infinitesimal rotations about the  $x_i$ -axis,  $i = 1, 2, 3$ , so that

$$\delta_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \delta_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \delta_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (3.17)$$

Then

$$[\delta_1, \delta_2] = \delta_3, \quad [\delta_2, \delta_3] = \delta_1, \quad [\delta_3, \delta_1] = \delta_2. \quad (3.18)$$

This can be expressed more succinctly by  $[\delta_i, \delta_j] = \epsilon_{ijk} \delta_k$ , where

$$\epsilon_{ijk} = \begin{cases} 1 & \text{for } (i, j, k) \text{ an even permutation of } (1, 2, 3) \\ -1 & \text{for } (i, j, k) \text{ an odd permutation of } (1, 2, 3) \\ 0 & \text{otherwise.} \end{cases} \quad (3.19)$$

The  $\delta_i$  are clearly linearly independent and so form a basis of  $\mathfrak{o}(3)$ . So if we write the most general element of  $\mathfrak{o}(3)$  as  $\mathbf{a} = a_1 \delta_1 + a_2 \delta_2 + a_3 \delta_3$  then the preceding equations for the brackets of the basis elements show that the Lie product in  $\mathfrak{o}(3)$

can be identified with the usual vector product,

$$[\mathbf{a}, \mathbf{b}] = \mathbf{a} \times \mathbf{b}. \quad (3.20)$$

Notice that this operation can also be described by thinking of  $\mathbf{a}$  as a matrix and  $\mathbf{b}$  as a vector and multiplying the vector  $\mathbf{b}$  by the matrix  $\mathbf{a}$ . For example, the fact that  $[\delta_1, \delta_2] = \delta_3$  can be expressed as

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (3.21)$$

### $e(3)$

Let  $E(3)$  denote the group of all Euclidean motions in three-dimensional space. So  $E(3)$  consists of all transformations of  $\mathbb{R}^3$  of the form

$$\mathbf{r} \mapsto R\mathbf{r} + \mathbf{v}, \quad (3.22)$$

where  $R \in O(3)$  and  $\mathbf{v} \in \mathbb{R}^3$ , in other words an orthogonal transformation followed by a translation. We can realize this transformation as matrix multiplication in four dimensions:

$$\begin{pmatrix} \mathbf{r} \\ 1 \end{pmatrix} \mapsto \begin{pmatrix} R & \mathbf{v} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{r} \\ 1 \end{pmatrix}, \quad (3.23)$$

so  $E(3)$  can be thought of as the group of all  $4 \times 4$  matrices of the form

$$\begin{pmatrix} R & \mathbf{v} \\ 0 & 1 \end{pmatrix}. \quad (3.24)$$

Therefore the Lie algebra  $e(3)$  can be identified with the algebra of all  $4 \times 4$  matrices of the form

$$\begin{pmatrix} \mathbf{a} & \mathbf{b} \\ 0 & 0 \end{pmatrix}, \quad (3.25)$$

with  $\mathbf{a} \in o(3)$  and  $\mathbf{b} \in \mathbb{R}^3$ . But recall from Eq. (3.20) that we have an identification of  $o(3)$  with  $\mathbb{R}^3$ . Therefore we can identify the six-dimensional algebra  $e(3)$  as a *vector space* with

$$o(3) \oplus o(3). \quad (3.26)$$

If  $[\cdot, \cdot]_{o(3)}$  denotes the bracket in the Lie algebra  $o(3)$  then the Lie bracket in  $e(3)$ , which is just the commutator of  $4 \times 4$  matrices restricted to matrices in  $e(3)$  as

above, is

$$[(\mathbf{a}_1, \mathbf{b}_1), (\mathbf{a}_2, \mathbf{b}_2)] = ([\mathbf{a}_1, \mathbf{a}_2]_{\mathfrak{o}(3)}, [\mathbf{a}_1, \mathbf{b}_2]_{\mathfrak{o}(3)} - [\mathbf{a}_2, \mathbf{b}_1]_{\mathfrak{o}(3)}). \quad (3.27)$$

The bracket of two elements of the form  $(\mathbf{a}, 0)$  is just the  $\mathfrak{o}(3)$  bracket in the  $\mathbf{a}$  position, that is

$$[(\mathbf{a}, 0), (\mathbf{b}, 0)] = ([\mathbf{a}, \mathbf{b}]_{\mathfrak{o}(3)}, 0). \quad (3.28)$$

The bracket of an  $\mathbf{a}$  and a  $\mathbf{b}$  is the  $\mathfrak{o}(3)$  bracket in the  $\mathbf{b}$  position, that is

$$[(\mathbf{a}, 0), (0, \mathbf{b})] = (0, [\mathbf{a}, \mathbf{b}]_{\mathfrak{o}(3)}). \quad (3.29)$$

Finally, the bracket of two  $\mathbf{b}$ s is zero:

$$[(0, \mathbf{b}_1), (0, \mathbf{b}_2)] = 0. \quad (3.30)$$

#### $\mathfrak{o}(4)$

This is the algebra of all antisymmetric  $4 \times 4$  matrices, so a basis is given by

$$\begin{aligned} \delta_1 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & \delta_2 &= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & \delta_3 &= \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \\ \omega_1 &= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, & \omega_2 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, & \omega_3 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \end{aligned} \quad (3.31)$$

and we write a general element of  $\mathfrak{o}(4)$  as  $a_i \delta_i + b_i \omega_i$ ,  $i = 1, 2, 3$ , or as

$$\begin{pmatrix} \mathbf{a} & \mathbf{b} \\ -\mathbf{b}^T & 0 \end{pmatrix}, \quad (3.32)$$

with  $\mathbf{a} \in \mathfrak{o}(3)$  and  $\mathbf{b} \in \mathbb{R}^3$ . Once again, this six-dimensional Lie algebra can be identified as a vector space with  $\mathfrak{o}(3) \oplus \mathfrak{o}(3)$ . The bracket of two  $\mathbf{a}$ s is the same as before, as is the bracket of an  $\mathbf{a}$  and a  $\mathbf{b}$ . What is new is the bracket of two  $\mathbf{b}$ s. In the algebra  $\mathfrak{o}(4)$  we have

$$[(0, \mathbf{b}_1), (0, \mathbf{b}_2)] = ([\mathbf{b}_1, \mathbf{b}_2]_{\mathfrak{o}(3)}, 0). \quad (3.33)$$

$\mathfrak{o}(3,1)$

This is the algebra of  $4 \times 4$  matrices of the form

$$\begin{pmatrix} \mathbf{a} & \mathbf{b} \\ \mathbf{b}^T & 0 \end{pmatrix}, \quad (3.34)$$

with  $\mathbf{a} \in \mathfrak{o}(3)$  and  $\mathbf{b} \in \mathbb{R}^3$ . It can be shown that this is the Lie algebra of the Lorentz group — the group of all linear transformations of  $\mathbb{R}^4$  that preserve the quadratic form

$$x_1^2 + x_2^2 + x_3^2 - x_4^2. \quad (3.35)$$

Once again the bracket between two  $\mathbf{a}$ s and an  $\mathbf{a}$  and a  $\mathbf{b}$  is as before. But now

$$[(0, \mathbf{b}_1), (0, \mathbf{b}_2)] = (-[\mathbf{b}_1, \mathbf{b}_2]_{\mathfrak{o}(3)}, 0). \quad (3.36)$$

In all three cases,  $\mathfrak{e}(3)$ ,  $\mathfrak{o}(4)$ ,  $\mathfrak{o}(3, 1)$ , the Lie algebra decomposes as a vector space direct sum

$$\mathcal{G} = k + p, \quad (3.37)$$

with

$$[k, k] \subset k, \quad [k, p] \subset p, \quad \text{and} \quad [p, p] \subset k. \quad (3.38)$$

In these three cases  $k = p = \mathfrak{o}(3)$  as vector spaces, and the  $[k, k]$  and  $[k, p]$  brackets are the  $\mathfrak{o}(3)$  brackets. The bracket of  $p$  back into  $k$  is given by  $\lambda[\cdot, \cdot]_{\mathfrak{o}(3)}$ , where  $\lambda = 1$  for  $\mathfrak{o}(4)$ ,  $\lambda = 0$  for  $\mathfrak{e}(3)$ , and  $\lambda = -1$  for  $\mathfrak{o}(3, 1)$ .

It is notable that in the  $\mathfrak{o}(4)$  case we have  $k = p$  as vector spaces, and when we make this vector space identification all three brackets are the same: The subspaces

$$\Delta = \{(\mathbf{a}, \mathbf{a})\} \quad \text{the diagonal} \quad (3.39)$$

and

$$\Delta^T = \{(\mathbf{b}, -\mathbf{b})\} \quad \text{the antidiagonal} \quad (3.40)$$

are both subalgebras isomorphic to  $k$  and we have the *Lie algebra* direct sum decomposition

$$\mathcal{G} = \Delta \oplus \Delta^T. \quad (3.41)$$

Thus  $\mathfrak{o}(4)$  is Lie algebra isomorphic to  $\mathfrak{o}(3) \oplus \mathfrak{o}(3)$ . This identification in Lie theory has remarkable physical consequences as will become apparent in Chapter 8.

### 3.3 Poisson Brackets

The implementation of symmetries is seen most clearly in the Hamiltonian formulation of classical mechanics. In this formulation an observable is a function on phase space. In addition to the usual addition and multiplication, the space of functions on phase space has another binary operation known as the *Poisson bracket*: Given two functions,  $f$  and  $g$ , their Poisson bracket  $\{f, g\}$  is a third function on phase space, and this operation satisfies the following rules:

- (a)  $\{f, g\}$  is bilinear in  $f$  and  $g$ ;
- (b)  $\{, \}$  is antisymmetric, that is  $\{g, f\} = -\{f, g\}$ ;
- (c) Jacobi's identity:  $\{f, \{g, h\}\} = \{\{f, g\}, h\} + \{g, \{f, h\}\}$ ; and
- (d)  $f$  acting on  $gh$  satisfies the Leibniz rule:  $\{f, gh\} = \{f, g\}h + g\{f, h\}$ .

The first three axioms are just the axioms for a Lie algebra: The space of functions on phase space form a Lie algebra under the Poisson bracket. Axiom (d) ties the Poisson bracket in with usual multiplication. It says that the Poisson bracket acts as a *derivation*. A commutative algebra  $\mathcal{A}$  having a bracket satisfying the above axioms is called a *Poisson algebra*.

For example, the phase space  $X$  for a single classical particle moving in ordinary three-dimensional space is the six-dimensional space consisting of all possible positions and momenta. So  $X$  is six-dimensional, with coordinates  $(x_1, x_2, x_3, p_1, p_2, p_3)$ . The Poisson brackets of these coordinate functions are

$$\{x_i, x_j\} = \{p_i, p_j\} = 0 \quad \text{and} \quad \{x_i, p_j\} = \delta_{ij}, \quad \text{with } i, j = 1, 2, 3. \quad (3.42)$$

When these bracket relations are realized we say that the coordinates  $p_1, p_2, p_3$  are the *canonically conjugate* variables to  $x_1, x_2, x_3$ . Using the axioms we find

$$\{x_i, p_j^2\} = p_j \{x_i, p_j\} + \{x_i, p_j\} p_j = 2p_j \delta_{ij}, \quad (3.43)$$

and, by iteration,

$$\{x_i, p_j^n\} = n p_j^{n-1} \delta_{ij}. \quad (3.44)$$

Therefore

$$\{x_i, g\} = \frac{\partial g}{\partial p_i}, \quad (3.45)$$

and similarly

$$\{p_i, g\} = -\frac{\partial g}{\partial x_i}, \quad (3.46)$$

for any polynomial  $g = g(x, p)$ . We then have

$$\{f, g\} = \frac{\partial f}{\partial x_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x_i}, \quad (3.47)$$

for any pair of polynomials  $f$  and  $g$ . This is, in fact, the formula for the Poisson bracket of any pair of functions.

A transformation is called  $\phi$  *symplectic* if the induced transformation on functions

$$f \mapsto f \circ \phi^{-1}, \quad (3.48)$$

preserves the Poisson bracket, that is, if

$$\{f, g\} \circ \phi^{-1} = \{f \circ \phi^{-1}, g \circ \phi^{-1}\} \quad (3.49)$$

for all functions  $f$  and  $g$ . It turns out that every function  $f$  on phase space generates a (local) one-parameter group,  $\phi_t$ , of symplectic transformations such that

$$\{f, g\} = \left[ \frac{d}{dt} \right]_{t=0} g \circ \phi_{-t}. \quad (3.50)$$

So forming the Poisson bracket with  $f$  (on the left) is the infinitesimal symmetry associated to  $f$ . A function on phase space serves a double role: It is an observable, and it also determines an infinitesimal symmetry of the space of observables via the Poisson bracket.

Let  $\mathcal{G}$  be a Lie algebra. We say that we have a *Hamiltonian action* of  $\mathcal{G}$  on  $X$  if we are given a Lie algebra homomorphism  $\sigma : \mathcal{G} \mapsto \mathcal{A}$ , where  $\mathcal{A}$  denotes the space of functions on  $X$ . Thus  $\sigma$  assigns to each element  $\xi \in \mathcal{G}$  a function  $\sigma(\xi)$  on  $X$  and

$$\{\sigma(\xi), \sigma(\eta)\} = \sigma([\xi, \eta]) \quad (3.51)$$

for every  $\eta \in \mathcal{G}$ .

For example, consider the case of the phase space of a single free particle as above. Let  $\mathcal{G}$  be the Lie algebra consisting of all  $3 \times 3$  matrices under the commutator bracket, and define

$$\sigma(M) = -M_{ij}x_i p_j. \quad (3.52)$$

Equation (3.51) holds, since

$$\begin{aligned} \{\sigma(\xi), \sigma(\eta)\} &= M_{ij}N_{mn} \left( \frac{\partial(x_i p_j)}{\partial x_k} \frac{\partial(x_m p_n)}{\partial p_k} - \frac{\partial(x_i p_j)}{\partial p_k} \frac{\partial(x_m p_n)}{\partial x_k} \right) \\ &= M_{ij}N_{mn} (\delta_{ik}\delta_{nk}p_j x_m - \delta_{jk}\delta_{mk}x_i p_n) \end{aligned}$$



$$\begin{aligned}
&= M_{ij}N_{mi}p_jx_m - M_{im}N_{mn}x_ip_n \\
&= (NM)_{ij}x_ip_j - (MN)_{ij}x_ip_j = -[M, N]_{ij}x_ip_j = \sigma([\xi, \eta]).
\end{aligned} \tag{3.53}$$

Notice also that

$$\{\sigma(M), x_k\} = M_{ik}x_i \quad \text{and} \quad \{\sigma(M), p_k\} = -M_{kj}p_j. \tag{3.54}$$

So if we identify the function  $x_k$  with the  $k$ th basis element in  $\mathbb{R}^3$  then the first equation in (3.54) identifies the bracket with  $\sigma(M)$  with the matrix  $M_{ij}$  and so  $\sigma$  defines an isomorphism between the Lie algebra  $\mathfrak{gl}(3, \mathbb{R})$  and the subalgebra of  $\mathcal{A}$  consisting of all homogeneous polynomials of degree two, which are of degree one in  $x$  and degree one in  $p$ . For example, if  $L_3 = x_1p_2 - x_2p_1$  then

$$\{L_3, x_1\} = x_2, \quad \{L_3, x_2\} = -x_1, \quad \{L_3, x_3\} = 0, \tag{3.55}$$

and

$$\{L_3, p_1\} = p_2, \quad \{L_3, p_2\} = -p_1, \quad \{L_3, p_3\} = 0. \tag{3.56}$$

The first of these equations says that  $L_3$  acts on  $\mathbf{r}$  as an infinitesimal rotation about the  $x_3$ -axis. Let  $\mathfrak{o}(3) \in \mathfrak{gl}(3, \mathbb{R})$  be the Lie algebra of infinitesimal rotations and let  $L$  denote the restriction of  $\sigma$  to  $\mathfrak{o}(3)$ . Recall that  $\delta_3$  denotes infinitesimal rotation about the  $x_3$ -axis (with similar notation for  $\delta_1$  and  $\delta_2$ ) and then  $L_3 = L(\delta_3)$ .

Let us use  $\times$  to denote the vector product on  $\mathbb{R}^3$ . We have made the identification of  $\mathfrak{o}(3)$  with  $\mathbb{R}^3$  so that the Lie bracket is given by  $\times$ . That is, the elements of  $\mathfrak{o}(3)$  are regarded as vectors and the Lie bracket becomes the vector product. The elements of  $\delta_i$  then become the standard basis vectors. If we form the vector-valued function

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{3.57}$$

then under the identification of  $\mathfrak{o}(3)$  with  $\mathbb{R}^3$  we have, for any  $\xi \in \mathbb{R}^3$ ,

$$L(\xi) = \mathbf{L} \cdot \xi, \tag{3.58}$$

and (3.51) becomes

$$L([\xi, \eta]) = \{L(\xi), L(\eta)\}. \tag{3.59}$$

The function  $\mathbf{L}$  is called the *angular momentum*.

The time evolution of a mechanical system is the one-parameter group generated by the Hamiltonian  $H$ . The infinitesimal change in any observable  $f$

under this time evolution is thus given by  $\{H, f\}$ . We say that  $H$  is invariant under the action  $\sigma$  of the Lie algebra  $\mathcal{G}$  if

$$\{\sigma(\xi), H\} = 0 \quad (3.60)$$

for all  $\xi \in \mathcal{G}$ . This, by the antisymmetry of  $\{, \}$ , implies that  $\{H, \sigma(\xi)\} = 0$ . In other words, all the functions  $\sigma(\xi)$  are conserved quantities under the flow generated by  $H$ . Thus if  $H$  is rotationally invariant, this means that all the functions  $L(\xi)$ , or, what amounts to the same thing, each of the functions  $L_1, L_2, L_3$  are constant along the trajectories of  $H$ . In other words, the vector-valued function  $\mathbf{L}$  is constant. This is *the principle of conservation of angular momentum*.

Infinitesimal translation in the  $x_1$  direction acts on phase space by the Poisson bracket with  $p_1$ . Indeed,

$$\{p_1, x_1\} = -1, \quad \{p_1, x_2\} = \{p_1, x_3\} = \{p_1, p_i\} = 0, \quad i = 1, 2, 3. \quad (3.61)$$

Thus invariance of the Hamiltonian under the full translation group implies conservation of the vector-valued function  $\mathbf{p}$ . This is *the principle of the conservation of linear momentum*.

Thus invariance of the Hamiltonian under the full group of Euclidean motions containing all translations and rotations implies conservation of both linear and angular momentum. One of Galileo's principal revolutionary achievements was to replace the geocentric Aristotelian theory, which has an  $O(3)$  symmetry centered at the origin of the Earth, with the larger symmetry group  $E(3)$ . Indeed, it is easy to check that the map

$$(\mathbf{a}, \mathbf{b}) \mapsto \mathbf{a} \cdot \mathbf{L} + \mathbf{b} \cdot \mathbf{p} \quad (3.62)$$

gives a Hamiltonian action of  $e(3)$  on phase space.

### 3.4 The Inverse Square Law

In the problem of a particle moving under the influence of a central force we no longer have translational symmetry, but we retain rotational symmetry about the origin. We do not have  $\{H, \mathbf{p}\} = 0$ , but if the force is inversely proportional to the square of the distance we have the three conserved quantities  $\mathcal{A}$  of Eq. (2.22) in addition to the quantities  $\mathbf{L}$ . In the present formalism a quantity is conserved if its Poisson bracket with the Hamiltonian vanishes. We check that this is indeed the case. With

$$H = \frac{\mathbf{p}^2}{2m} - \frac{k}{r}, \quad (3.63)$$



we have

$$\begin{aligned}\{H, \mathcal{A}_i\} &= -\frac{1}{m}\epsilon_{ijk}\{1/r, p_j\}L_k - \frac{1}{m}p_j\{p_j, x_i/r\} \\ &= \frac{1}{m}(\epsilon_{ijk}x_jL_k/r^3 + p_i/r - x_i p_j x_j / r^3),\end{aligned}\quad (3.64)$$

Using Eq. (3.46), since  $\{L_i, f(r)\} = 0$  for  $f$  an arbitrary function of  $r$ . The first term is

$$\frac{1}{m}\epsilon_{ijk}\epsilon_{ksn}x_jx_s p_n / r^3 = \frac{1}{m}(\delta_{is}\delta_{jn} - \delta_{in}\delta_{js})x_jx_s p_n / r^3, \quad (3.65)$$

which cancels the second and third terms. We are using

$$L_i = \epsilon_{ijk}x_j p_k. \quad (3.66)$$

**Exercise 3.1** Prove  $\epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}$ .

**Exercise 3.2** Prove  $\epsilon_{ijk}\epsilon_{ijm} = 2\delta_{km}$ .

We want to see if these six quantities close to a Lie algebra. We still have

$$\{L(\xi), L(\eta)\} = L([\xi, \eta]) \quad (3.67)$$

as before. We also have

$$\{L(\xi), \mathcal{A}(\eta)\} = \mathcal{A}([\xi, \eta]), \quad (3.68)$$

which just says that  $\mathcal{A}$  transforms as a vector. Indeed,

$$\begin{aligned}\{L_i, \mathcal{A}_j\} &= \frac{1}{mk}\epsilon_{jsn}\{L_i, p_s L_n\} - \{L_i, x_j/r\} \\ &= \frac{1}{mk}\epsilon_{jsn}(\{L_i, p_s\}L_n + p_s\{L_i, L_n\}) - \{L_i, x_j\}\frac{1}{r} \\ &= \epsilon_{ijk}\left(\frac{(\mathbf{p} \times \mathbf{L})_k}{mk} - \frac{x_k}{r}\right) = \epsilon_{ijk}\mathcal{A}_k,\end{aligned}\quad (3.69)$$

We now wish to compute  $\{\mathcal{A}_i, \mathcal{A}_j\}$ . It is a somewhat lengthy calculation, but we go through it in detail because of the importance of the result, which will be needed in Chapter 8. We first calculate some Poisson brackets, which are used

below:

$$\begin{aligned}
 (mk)\{p_i, \mathcal{A}_j\} &= \epsilon_{jsn}\{p_i, p_s L_n\} - mk\{p_i, x_j/r\} \\
 &= \epsilon_{jsn}p_s\{p_i, L_n\} - mk\{p_i, x_j\}/r - mkx_j\{p_i, 1/r\} \\
 &= -\epsilon_{jsn}\epsilon_{niq}p_s p_q + mk\delta_{ij}/r - mkx_j x_i/r^3 \\
 &= (\delta_{jq}\delta_{si} - \delta_{ji}\delta_{sq})p_s p_q + mk\delta_{ij}/r - mkx_i x_j/r^3 \\
 &= p_i p_j - \mathbf{p}^2 \delta_{ij} + mk\delta_{ij}/r - mkx_i x_j/r^3, \tag{3.70}
 \end{aligned}$$

and

$$\begin{aligned}
 (mk)\{x_i/r, \mathcal{A}_j\} &= \epsilon_{jsn}\{x_i/r, p_s L_n\} = \epsilon_{jsn}(\{x_i, p_s L_n\}/r + \{1/r, p_s L_n\}x_i) \\
 &= \epsilon_{jsn}(p_s\{x_i, L_n\}/r + \{x_i, p_s\}L_n/r + \{1/r, p_s\}L_n x_i) \\
 &= \epsilon_{jsn}(-\epsilon_{nik}p_s x_k/r + \delta_{is}L_n/r - x_s x_i L_n/r^3) \\
 &= -(\delta_{ji}\delta_{sk} - \delta_{jk}\delta_{si})p_s x_k/r + \epsilon_{jin}L_n/r - \epsilon_{jsn}x_s x_i L_n/r^3 \\
 &= p_i x_j/r - \delta_{ij}x_m p_m/r - \epsilon_{ijm}L_m/r - \epsilon_{jmn}x_i x_m L_n/r^3. \tag{3.71}
 \end{aligned}$$

The latter yields, remembering that  $\mathbf{r} \cdot \mathbf{L} = 0$ , and using Exercises 3.1 and 3.2,

$$(mk)^2 \epsilon_{ijk}\{x_i/r, \mathcal{A}_j\} = -2mkL_k/r. \tag{3.72}$$

We are now ready to do the main calculation:

$$\begin{aligned}
 (mk)^2 \epsilon_{ijk}\{\mathcal{A}_i, \mathcal{A}_j\} &= (mk)\epsilon_{ijk}(\epsilon_{isn}\{p_s L_n, \mathcal{A}_j\} - (mk)\{x_i/r, \mathcal{A}_j\}) \\
 &= (mk)\epsilon_{ijk}(\epsilon_{isn}(p_s\{L_n, \mathcal{A}_j\} + \{p_s, \mathcal{A}_j\}L_n) \\
 &\quad - (mk)\{x_i/r, \mathcal{A}_j\}). \tag{3.73}
 \end{aligned}$$

We evaluate the separate terms:

$$\begin{aligned}
 \epsilon_{ijk}\epsilon_{isn}p_s\{L_n, \mathcal{A}_j\} &= \epsilon_{ijk}\epsilon_{isn}\epsilon_{njq}p_s \mathcal{A}_q \\
 &= \epsilon_{ijk}(\delta_{ij}\delta_{sq} - \delta_{iq}\delta_{sj})p_s \mathcal{A}_q = \epsilon_{ijk}p_i \mathcal{A}_j, \tag{3.74}
 \end{aligned}$$

and

$$\begin{aligned}
 (mk)\epsilon_{ijk}p_i \mathcal{A}_j &= \epsilon_{ijk}\epsilon_{jsq}p_i p_s L_q - (mk)\epsilon_{ijk}p_i x_j/r \\
 &= (\delta_{iq}\delta_{ks} - \delta_{is}\delta_{kq})p_i p_s L_q + (mk)L_k/r \\
 &= (-\mathbf{p}^2 + mk/r)L_k. \tag{3.75}
 \end{aligned}$$

Also

$$\begin{aligned}
 (mk)\epsilon_{ijk}\epsilon_{isn}\{p_s, \mathcal{A}_j\}L_n &= \epsilon_{ijk}\epsilon_{isn}(p_s p_j - \mathbf{p}^2 \delta_{sj} + mk \delta_{sj}/r \\
 &\quad - mk x_s x_j / r^3) L_n \\
 &= (\delta_{js} \delta_{kn} - \delta_{jn} \delta_{ks})(p_s p_j - \mathbf{p}^2 \delta_{sj} + mk/r \delta_{sj} \\
 &\quad - mk x_s x_j / r^3) L_n \\
 &= (-2p^2 + 2mk/r)L_k - (-\mathbf{p}^2 + mk/r)L_k \\
 &= (-\mathbf{p}^2 + mk/r)L_k.
 \end{aligned} \tag{3.76}$$

Combining these results, we get

$$\begin{aligned}
 (mk)^2 \epsilon_{ijk} \{\mathcal{A}_i, \mathcal{A}_j\} &= [(-\mathbf{p}^2 + mk/r) + (-\mathbf{p}^2 + mk/r) + 2mk/r] L_k \\
 &= -2(\mathbf{p}^2 - 2mk/r) L_k = -4mHL_k.
 \end{aligned} \tag{3.77}$$

Multiply by  $\epsilon_{ijk}$  to finally get

$$(mk)^2 \epsilon_{ijk} \epsilon_{mnk} \{\mathcal{A}_m, \mathcal{A}_n\} = 2(mk)^2 \{\mathcal{A}_i, \mathcal{A}_j\} = -4m\epsilon_{ijk} H L_k, \tag{3.78}$$

and

$$\{\mathcal{A}_i, \mathcal{A}_j\} = \epsilon_{ijk} \left( \frac{-2H}{mk^2} \right) L_k. \tag{3.79}$$

The occurrence of  $H(\mathbf{r}, \mathbf{p})$  in the last equation prevents the quantities  $L_i$  and  $\mathcal{A}_i$  from closing to a Lie algebra on the whole phase space. But when the motion is in a fixed orbit  $H(\mathbf{r}, \mathbf{p}) = E$ , with  $E$  a constant energy. We can then divide the phase space into three sets, the two open regions where  $H > 0$  and  $H < 0$ , and their common boundary where  $H = 0$ . In the region where  $H > 0$  we can rescale  $\mathcal{A}$  by  $2H/mk^2$  to get an  $\mathfrak{o}(3, 1)$  algebra. In the region where  $H < 0$  we can rescale by  $-2H/mk^2$  to get an  $\mathfrak{o}(4)$  algebra.

That is, we define

$$A = \mathcal{N} \mathcal{A}, \tag{3.80}$$

where

$$\mathcal{N}^{-2} = -\frac{2H}{mk^2}, \tag{3.81}$$

to get

$$\{L_i, L_j\} = \epsilon_{ijk} L_k, \quad \{L_i, A_j\} = \epsilon_{ijk} A_k, \quad \{A_i, A_j\} = \epsilon_{ijk} L_k. \tag{3.82}$$

This shows that the quantities  $L_i$  and  $A_i$  close to form an  $\mathfrak{o}(4)$  Lie algebra.

We can use the Lie algebra isomorphism of  $\mathfrak{o}(4)$  with  $\mathfrak{o}(3) \oplus \mathfrak{o}(3)$  to form the direct sum of two  $\mathfrak{o}(3)$  algebras. Define

$$M_i = L_i + A_i, \quad N_i = L_i - A_i. \quad (3.83)$$

Then the Poisson structure becomes

$$\{M_i, M_j\} = \epsilon_{ijk} M_k, \quad \{N_i, N_j\} = \epsilon_{ijk} N_k, \quad \{M_i, N_j\} = 0. \quad (3.84)$$

We have shown that a force which is inversely proportional to the square of the distance between the particles leads, in the case of bound states, to six conserved quantities which form, when properly normalized, the generators of an  $\mathfrak{so}(4)$  algebra that acts on the functions of phase space. This result, which appears here in a somewhat abstract form, gives rise to physical results when applied to the spectrum of hydrogen in Chapter 8.

### Notes on Chapter 3

This review of Hamiltonian mechanics is standard, and can be found in any good text on classical mechanics. It is included here to make the treatment self-contained. The same is true for the relation between Lie groups and Lie algebras. More information can be found in Weaver and Sattinger [WS10], or Marsden and Ratiu [MR99]. We follow here the treatment of Guillemin and Sternberg [GS90]. The calculation of the Poisson bracket between the components of the Laplace vector is the classical version of the calculation of the corresponding commutator by Sudbery [Sud86].

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## Chapter 4

### From Solar Systems to Atoms

#### 4.1 Rutherford Scattering

*“It was quite the most incredible event that has ever happened to me in my life. It was almost as incredible as if you fired a 15-inch shell at a piece of tissue paper and it came back and hit you.”*

Lord Rutherford, quoted in *Rutherford and the Nature of the Atom*, E. N. da C. Andrade, Heinemann, London, 1964.

In 1897 J. J. Thompson measured the mass-to-charge ratio of the electron. In 1902 Lord Kelvin proposed that the atom consisted of a sphere of positive charge in which the electrons were embedded. In 1906 W. Thompson reasoned that the number of electrons in an atom was approximately equal to the atom's atomic weight. On this basis, there would be only one electron in the hydrogen atom.

In 1911 Rutherford [Rut11] established, from the data of scattering experiments with alpha particles impinging on gold folie, that the positive charge in the atom is concentrated in a nucleus 10,000 times smaller than the atom itself. This nucleus also carries most of the mass of the atom. This was the background on which Bohr [Boh13] developed his model of the hydrogen atom in 1913. The electron and its nucleus form a two-body system, with an electron mass that is negligible in comparison to the mass of the nucleus. Hence one has a point electron moving in the Coulomb potential of a nucleus of charge one.

To understand Rutherford's reasoning we shall derive his formula for scattering. In this derivation we shall again make use of the Laplace vector of the system. We do this in order to get some practice with the application of the Laplace vector, and also because the formula is of paramount importance on the road to understanding atomic physics.

## 4.2 Conservation of the Laplace Vector

We consider impinging particles of charge  $e$ , and as target a nucleus of charge  $Ze$ . The central force is repulsive, and  $k$  in Eq. (2.17) is negative,  $k = -|k| = -Z\alpha$ . Then the Laplace vector is

$$\mathcal{A} = -\frac{(\mathbf{p} \times \mathbf{L})}{Z\alpha m} - \hat{\mathbf{r}}. \quad (4.1)$$

The scattering process is described as in Figure 4.1. Long before the collision takes place the initial impulse of a particle in the beam is  $\mathbf{p}_i = mv_0\mathbf{e}_i$ , where  $v_0$  is the velocity of the incoming particle and  $\mathbf{e}_i$  is a unit vector in the direction of the incoming velocity. The final velocity is  $\mathbf{p}_f = mv_0\mathbf{e}_f$ , with the same velocity  $v_0$  (the process is *elastic*) and  $\mathbf{e}_f$  is a unit vector in the direction of the outgoing velocity.  $\mathbf{L}_i = \mathbf{L}_f = mv_0b\hat{\mathbf{k}}$ , where  $\mathbf{L}$  is the conserved angular momentum, and  $\hat{\mathbf{k}}$  is a unit vector pointing up through the page, perpendicular to the scattering plane.  $b$  is the *impact parameter*, the distance that the incoming particle would pass by the point target in the absence of interaction. The initial incoming direction is  $\hat{\mathbf{r}}_i = -\mathbf{e}_i$ , and the final outgoing direction  $\hat{\mathbf{r}}_f = \mathbf{e}_f$ .

The initial Laplace vector is

$$\mathcal{A}_i = -\left(\frac{mv_0^2}{Z\alpha}\right)b\mathbf{n}_i + \mathbf{e}_i, \quad (4.2)$$

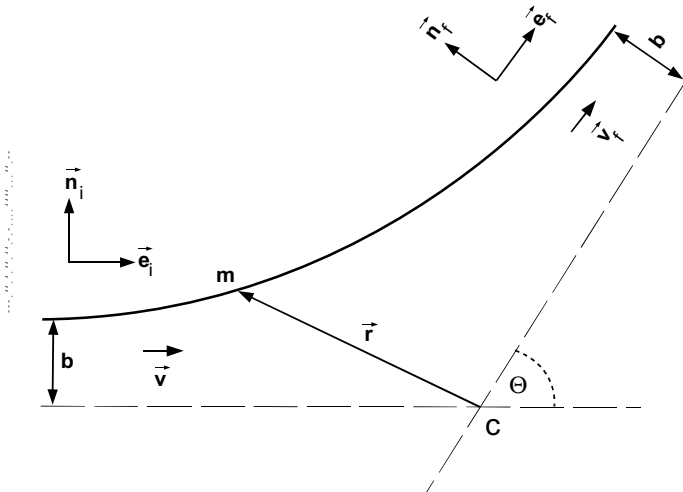


Figure 4.1. The incoming and outgoing directions and the scattering angle.

where  $\mathbf{n}_i$  is the unit vector in Figure 4.1 perpendicular to  $\mathbf{e}_i$  and in the scattering plane. The final Laplace vector is

$$\mathcal{A}_f = - \left( \frac{mv_0^2}{Z\alpha} \right) \mathbf{n}_f - \mathbf{e}_f, \quad (4.3)$$

where  $\mathbf{n}_f$  is the unit vector perpendicular to  $\mathbf{e}_f$  and in the scattering plane.

Conservation of the Laplace vector yields

$$\mathcal{A}_i \cdot \mathbf{e}_i = \mathcal{A}_f \cdot \mathbf{e}_i. \quad (4.4)$$

With  $(\mathbf{e}_f \cdot \mathbf{e}_i) = \cos \theta$ , where  $\theta$  is the scattering angle, and  $(\mathbf{n}_f \cdot \mathbf{e}_i) = \cos(\pi/2 + \theta) = -\sin \theta$ , this leads to

$$Z\alpha = mv_0^2 b \sin \theta - Z\alpha \cos \theta. \quad (4.5)$$

Rearranging this gives a relation between  $b$  and  $\theta$ ,

$$\tan(\theta/2) = \frac{Z\alpha}{mv_0^2 b}, \quad (4.6)$$

and this enables us to calculate the scattering angle for any impact parameter.

### 4.3 The Differential Cross Section

The differential scattering cross section is defined in terms of the number of particles scattered into the shaded band  $2\pi d\theta$  in Figure 4.2. From the figure this is the same as the number of particles incident on the area  $2\pi b db$ , and the differential cross

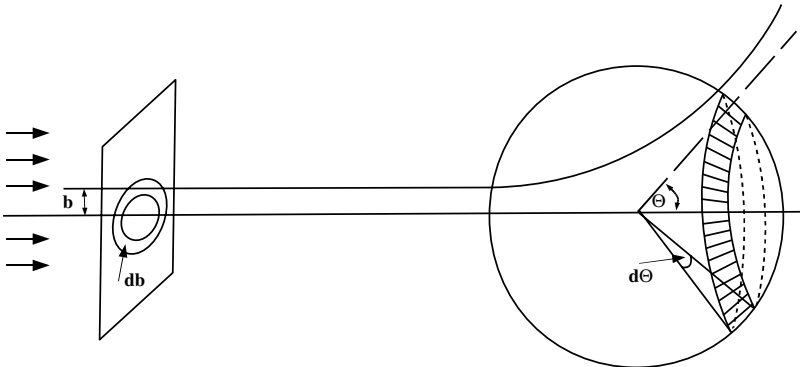


Figure 4.2. Scattering of an incident beam of particles by a center of force.

section is

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin \theta} \left| \frac{db}{d\theta} \right|. \quad (4.7)$$

We calculate, from Eq. (4.6),

$$\left| \frac{db}{d\theta} \right| = \frac{Z\alpha}{2mv_0^2 \sin^2(\theta/2)}. \quad (4.8)$$

Therefore we obtain *Rutherford's scattering formula*:

$$\frac{d\sigma}{d\Omega} = \frac{(Z\alpha)^2}{4(mv_0^2)^2 \sin^4(\theta/2)}. \quad (4.9)$$

The result for the Thompson atom, which involves multiple scattering, decreases much more rapidly than the characteristic  $\sin^{-4}(\theta/2)$  of Rutherford's formula. This is the reason for Rutherford's surprise, noted earlier. Together with his associates, Geiger and Marsden, he verified the formula in great detail, including its proportionality to  $Z^2$ , and the inverse squared proportionality to the kinetic energy of the incoming particles. The formula was also found to be accurate down to small distances, and the finite size of the nucleus, at which deviations from the formula were observed, was around  $10^{-14}m = 10$  Fermi for an aluminium foil. The success of the formula proved the correctness of the assumptions on which it is based, and established the solar system model for atoms.

## Notes on Chapter 4

Rutherford scattering is analyzed using the Laplace vector by Basano and Bianchi [BB80], and in textbooks on classical mechanics; see, for example, Poole, Goldstein and Safko [PGS01].

## Chapter 5

### The Bohr Model

*“The spectrum of the hydrogen atom has proved to be the Rosetta stone of modern physics.”*

Theodor W. Hänsch, Arthur L. Schawlow, and George W. Series, in *Rev. Mod. Phys.* 54, p. 697 (1982).

#### 5.1 Spectroscopic Series

Balmer published in 1885 an empirical formula for the frequencies of the spectral lines of the hydrogen spectrum in the visible region,

$$h\nu = R_{\infty} \left( \frac{1}{4} - \frac{1}{N^2} \right), \quad (5.1)$$

with  $N = 3, 4, 5, 6$ . We have used here a modern notation for the constants, with  $h$  the constant later discovered by Planck [Pla00],  $\nu$  the frequency of the light emitted, and  $R_{\infty}$  the Rydberg constant.

This provided the key for the Bohr model of the hydrogen atom. Subsequently the Balmer formula was generalized to further series, these were found *after* Bohr had proposed his model; see Table 5.1 and Figure 5.1.

#### 5.2 The Postulates of the Model

In 1913 Niels Bohr presented a model of the hydrogen atom [Boh13], which quantitatively explained the spectroscopic measurements to the accuracy which was obtainable at that time. He based his model on the following postulates:

1. An electron in a hydrogen atom moves under the influence of an attractive Coulomb potential between the electron and the nucleus according to the laws of classical mechanics (i.e., in particular in circular orbits).
2. Quantization condition: Instead of the infinity of orbits possible in classical mechanics, it is only possible for an electron to move in an orbit for which its orbital angular momentum  $L$  is an integral number.