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Research Report

A Computer Gallery of Mathematical Physics—A Course Outline

March 5th, 1985

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Abstract

A sampler of the fundamental equations of mathematical physics is presented, by means of computer programs which provide working models of interesting physical phenomena, including

- a satellite going around the Earth according to Newton,
- the propagation of an electromagnetic wave according to Maxwell,
- the same satellite going around the Earth according to Einstein,
- an electron moving in a one-dimensional potential according to Schrödinger, and
- sums over all histories according to Feynman.

These computer programs are like experimental laboratories in which one can play with physical phenomena, and most of them generate motion pictures of the simulated happenings, which helps to make these exotic phenomena more familiar and understandable.

The programs are presented in APL2, and each is less than a page long, showing how close APL is to the mathematics of general relativity and quantum mechanics.

Our intent is to transmit some of the basic ideas of mathematical physics to people who know little physics or mathematics, but who feel comfortable on the computer. This exposition, however, is for physicists who may be interested in using it as the basis for a course.

Preface

This "computer gallery" is an attempt to bring outsiders within touching distance of man's major achievements in his effort to understand the physical universe. Einstein and Infeld's book *The Evolution of Physics* does a marvelous job of explaining the major themes of physical theory to the general public without the use of mathematics. As its authors point out, *The Evolution of Physics* is not as easy to read as a novel. Nevertheless, it covers mechanics, electrodynamics, general relativity and quantum mechanics, the full range of fundamental physics, without requiring any previous knowledge of physics, and without more mathematics than is used at the checkout counter of a supermarket. Reading their book is a marvelous experience. And it is amazing to think that Einstein was personally involved in creating much of the physical theory described in his book.

Another classic in the popularization of science is Feynman's Messenger lectures on *The Character of Physical Law*, which was filmed by the BBC and later transcribed into an MIT Press paperback. As Feynman points out in these lectures, nature seems to behave in an essentially abstract mathematical manner; one cannot open the hood and expose the hidden mechanism of gears and belts. It is not really possible to appreciate the major aspects of the behavior of the physical universe, without the use of substantial amounts of mathematics.

This effort is also based on the premise that the fundamental ideas of physics are simple and beautiful, and can be appreciated by a large public. The major obstacle is not the difficulty of the concepts, but rather the unfamiliar mathematical vocabulary employed in formulating them. In their explanation of Newtonian physics, Einstein and Infeld get around this obstacle by explaining the basic concepts of the differential and integral calculus in intuitive physical terms without using the usual forbidding mathematical notation. Later they practically formulate in words Maxwell's partial differential equations for the electromagnetic field.

The usual path that leads from the popularizations of Einstein and Infeld and Feynman to within touching distance of the great intellectual poems of physical theory, is to pursue a course of study of several years duration, and to work one's way through a large number of textbooks, textbooks which must be diligently studied, one by one, in the proper order. It seems unfair to deprive those of us who cannot do this of the pleasure of being on intimate terms with so much beauty. Here we try to provide a short cut. Of course, the contents of years of study cannot be poured into one booklet. We concentrate on five major triumphs of mathematical physics, associated with the names of Newton, Maxwell, Einstein, Schrödinger, and Feynman, which illustrate major currents of physical thought, major themes, major styles in physical theory. And the attempt is made to achieve precision notwithstanding the mathematical barrier, by presenting the mathematics on the computer, rather than in traditional mathematical notation. Computer programming is a mathematical language that is rapidly becoming more widespread than traditional mathematics, due to the dramatic advent of the era of personal computing.

This "gallery" may be regarded as a mathematical appendix to Einstein and Infeld's popularization, in which computational working models are provided to illustrate the fundamental physical principles discussed by them. In each case we also indicate appropriate readings for students that help to explain the programs.

I would like to thank Neil Patterson and Robert Bernstein for their enthusiastic support and encouragement, and I am grateful to IBM's Research Division for giving me a sabbatical to work on this project, and to the Theoretical Physics Group of the Physical Sciences Department for its hospitality. The help of members of the Theoretical Physics Group has been invaluable, and I am especially indebted to Gordon Lasher, Bruce Elmegreen, Martin Gutzwiller, Philip Seiden, and Donald Weingarten, and also to Larry Schulman of the Technion in Haifa, who visited this group the summer of 1984. I am grateful to Donald Orth and Norman Brenner for their help with APL2. Finally, I want to thank for their patience and perseverance those who attended a course on this material given at the IBM Thomas J. Watson Research Center in the fall of 1984.

CONTENTS

Introduction

Before leaping into the details and the computer programs, we would like to summarize the personalities of the five pieces of physics we shall present.

The first major step in physical theory was due to Newton. He discovered rules for calculating planetary motion. In Chapter 1 we shall consider a model solar system, consisting of a finite number N of point masses interacting with each other via gravitational attraction. The physical state of this system is described by $7N$ real numbers giving the masses and the current positions and velocities of the N bodies. The force acting on a particle is the sum of the forces on it exerted by each of the other particles. And the force one particle exerts on another is proportional to the product of their masses and inversely proportional to the square of the distance between them. A force acting on a particle has the effect of producing an acceleration, that is, a change in its velocity, which is proportional to the force and inversely proportional to the mass of the particle.

These laws formulated by Newton gave rise to the so-called mechanical world view. There are a number of remarkably strange features of Newton's laws. Some of these problems were known to Newton himself and upset his contemporaries, and others later troubled Mach and were elucidated by Einstein. The major cause for amazement that the world runs this way is concerned with "action at a distance." How can two gravitating bodies far away from each other have an instantaneous effect upon one another, without something propagating through the space between them at finite speed? This objection seems quite reasonable, but Newton's laws postulate instantaneous action at a distance. And Feynman emphasizes another troubling aspect of Newton's laws, namely their abstract mathematical nature and the lack of a mechanism. "Does each planet measure the distance to its neighbors with a ruler and then use an internal computer to calculate the square of this distance?" he asks. Another conceptual difficulty is concerned with the fact that real numbers are employed in describing the physical state of a planetary system. Real numbers in principle contain an infinite amount of information, but no one has ever measured any physical quantity with more than about a dozen digits of precision, and floating point numbers in the computer usually only have about a half dozen or a dozen digits of precision.

The next major step forward in physical theory was from action at a distance to field theories, in which effects propagate locally and at finite speed throughout an extended region of space in which a field resides. In Chapter 2 we shall give a computer model of a piece of electromagnetic field. Now the mathematical framework consists of a cube in three dimensional space, and each point within it is associated with two vectors or arrows. Each vector may be represented by a triple of real numbers. One of the two vectors gives the magnitude and direction of the electrical field at that point, and the other gives the magnitude and direction of the magnetic field. Just as real numbers with infinite precision cannot be handled on the computer, neither can the infinity of interior points of a cube. So instead we consider an $N \times N \times N$ lattice of points. Each point affects its nearest neighbors, which in turn affect their neighbors, and so on, and this gives rise to light waves and radio signals. $2N^3$ vectors and $6N^3$ numbers define the state of the field.

There are a number of serious problems with Maxwell's equations. One problem, pointed out by quantum theory, is that electromagnetic waves also manifest a particle-like behavior called photons, particularly evident in hard X-rays and gamma rays. The version of Maxwell's equations we present is called the vacuum field equations, because it describes electromagnetic waves propagating in a vacuum. There are no sources of the fields. And the electron turns out to be a very troublesome field source, because it seems to be a perfect mathematical point. This unfortunately implies that an infinite amount of energy is stored in the electromagnetic field which surrounds it. Feynman emphasizes in *The Feynman Lectures on Physics* that this problem has never really been solved, not even in quantum field theory. Problems like this lead some people to suspect that perhaps it is not really the case that space and time are infinitely divisible and flow continuously. Perhaps space and time are discrete and come in minimum units or quanta

From Maxwell's vacuum field equations, we pass in Chapter 3 to Einstein's field theory of gravitation. In this theory gravity is achieved by a field of local effects rather than by action at a distance.

Einstein's theory predicts gravity waves, but so far these remain undetected. The protagonist is now a four dimensional manifold, the space-time continuum, which is curved or bent. Gravity waves are ripples in the curvature of space-time. Light and small test particles go as straight as they can through this curved medium, on what are called geodesics, which we show how to calculate. We also present Einstein's field equations in the form of a computer program which checks whether the way space-time is bent is okay or not, in a universe that is entirely empty except for a single point mass. This is the famous Schwarzschild solution describing a black hole and its event horizon.

In Chapter 4 we leave classical physics for quantum physics, a strange world full of probability waves propagating in many dimensional phase spaces, and interfering constructively and destructively with each other. Usually probabilities are real numbers between zero and one. Probability zero means impossible, and probability one means certain. The kind of probability which appears in quantum mechanics is very strange indeed, for it is a complex number, whose magnitude or size is proportional to the traditional probability or degree of propensity, but whose direction represents the phase of a wave. To distinguish them from normal probabilities, the complex-valued probabilities occurring in quantum physics are called probability amplitudes. Normally, if there are two different ways in which something can occur, then the overall probability of occurrence is the sum of the individual probabilities, and is greater than either one of them. But in quantum physics the situation is quite different. If two probability amplitudes that are added together have the same magnitude but opposite directions, then they cancel out and give a zero overall probability of occurrence. And the hydrogen atom according to Schrödinger's equation is a kind of musical instrument, whose discrete spectrum of energy levels corresponds to the different frequencies of sound generated by the instrument. It consists of a central proton surrounded by waves giving the probability amplitude that the electron is at any given location.

Finally, in Chapter 5 we consider Feynman path integrals and the quantum theory of fields. Here is our computer model for an electromagnetic field: The setting is now a space-time cube, represented as an $N \times N \times N \times N$ lattice of N^4 points. The electromagnetic field is not the primary object. Instead it results from a gauge or phase field. The gauge field is represented by angles of rotation specified on each of the links connecting adjacent points in the lattice, and there are $4N^4$ of these links. Thus it is necessary to specify $4N^4$ angles in order to specify a particular gauge field configuration history or path. In the Feynman path integral formulation of quantum mechanics, one calculates probabilities for experimental results according to the following prescription: a physical system may go along any path it likes, in fact it goes along all possible paths! Feynman gives a formula for calculating how much each path contributes to the overall probability, and how different paths interfere constructively and destructively with each other. It is really amazing that the world behaves in this bizarre fashion. This is closely related to the "many worlds" interpretation of quantum mechanics.

The latest efforts in the direction of a unified field theory, called non-abelian gauge theories, are similar to the model that we have just described. The principal innovation is that they involve a richer notion of "phase" than before. For example, instead of the rotations of a circle, one may consider the rotations of a multi-dimensional sphere.

Now for the details.

1. Action at a Distance: Newton's Law of Gravitation

Readings

- Einstein & Infield, Chapter 1, "The Rise of the Mechanical View."
- PSSC *Physics*, for the formulas for centrifugal force and gravitational potential energy

Newton—Orbits

```
        )LOAD NEWTON
SAVED 1985-01-08 19.04.15 (GMT-5) 2727K(2695K)

        ∇NEWTON[⎕]∇
[ 0]     NEWTON
[ 1]     ⎕IO←0
[ 2]     BODIES←2
[ 3]     ORBIT←50 50ρ' '
[ 4]     G←.667E¯10
[ 5]     T←0
[ 6]     DELT←60
[ 7]     M←6E24 10
[ 8]     V←X←BODIES 3ρ0
[ 9]     X[1;0]←1E7
[10]     V[1;1]←6E3
[11]     STEP←1
[12]    LOOP:
[13]     F←(⍳BODIES)∘.FORCE⍳BODIES
[14]     A←⊃(+/F)÷M
[15]     V←V+A×DELT
[16]     X←X+V×DELT
[17]     T←T+DELT
[18]     DRAW
[19]     →((12×15)≥STEP←STEP+1)/LOOP

        ∇FORCE[⎕]∇
[0]     F←I FORCE J ⍝ FORCE EXERTED ON BODY I BY BODY J
[1]     F←3ρ0
[2]     →(I=J)/0
[3]     DELX←X[J;]-X[I;]
[4]     R←(+/DELX*2)*.5
[5]     F←(G×M[I]×M[J]÷R*2)×(DELX÷R)

        ∇DRAW[⎕]∇
[0]     DRAW
[1]     ORBIT[25+⌊X[0;0]÷5E5;25+⌊X[0;1]÷5E5]←'E'
[2]     ORBIT[25+⌊X[1;0]÷5E5;25+⌊X[1;1]÷5E5]←'*'
[3]     →(0≠15|STEP)/0
[4]     ' '
[5]     'TIME IN HOURS = ',⍕T÷60×60
[6]     FRAME ORBIT

        ∇FRAME[⎕]∇
[0]     FRAME PIC
[1]     '|',('-',[0]PIC,[0]'-'),'|'
```

The program *Newton* provides a working model of a "solar system." It does planetary orbit calculations for point masses, according to Newton's laws:

$$F = m\,a$$

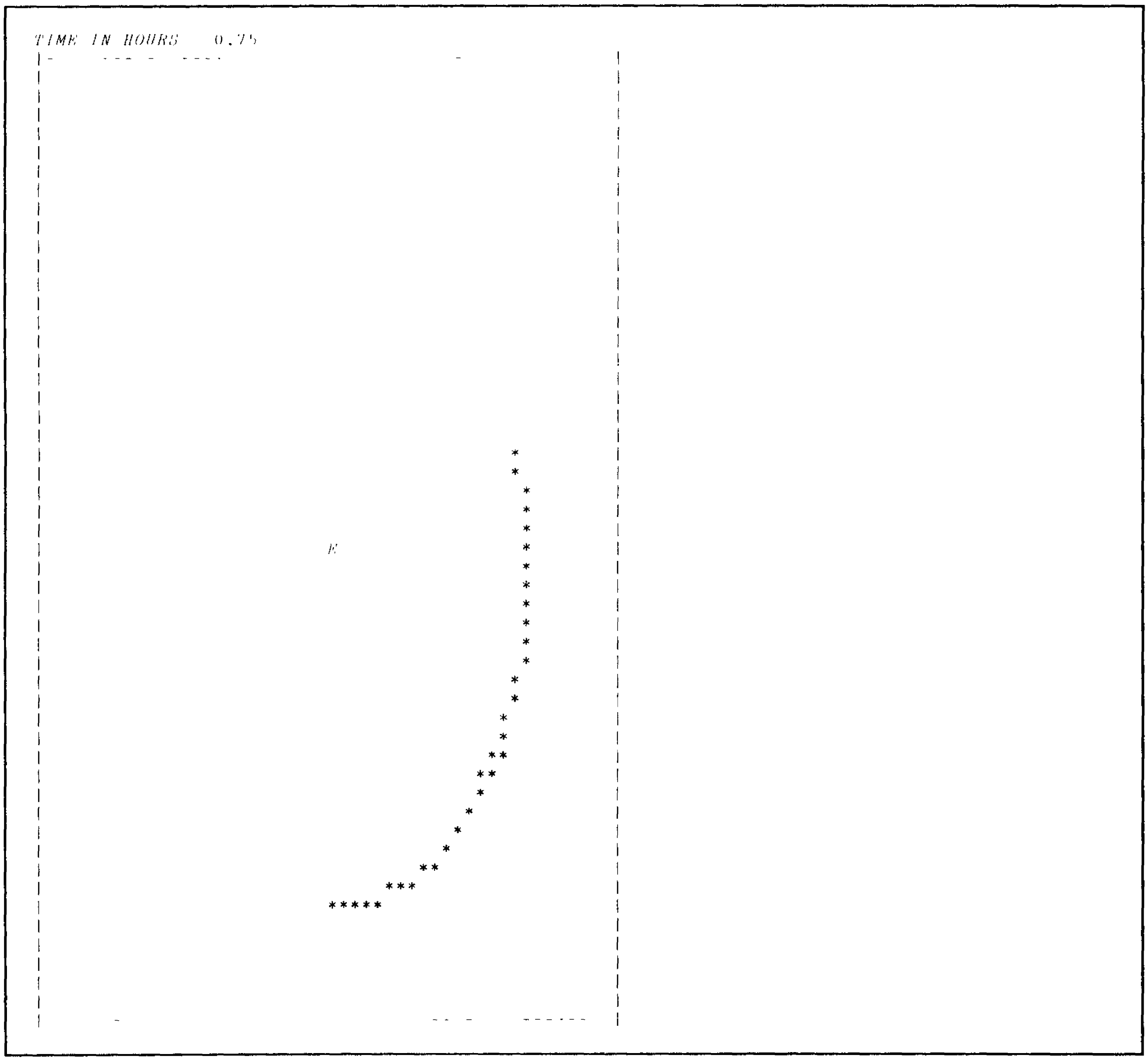
$$F = G\,\frac{m\,m'}{r^2}$$

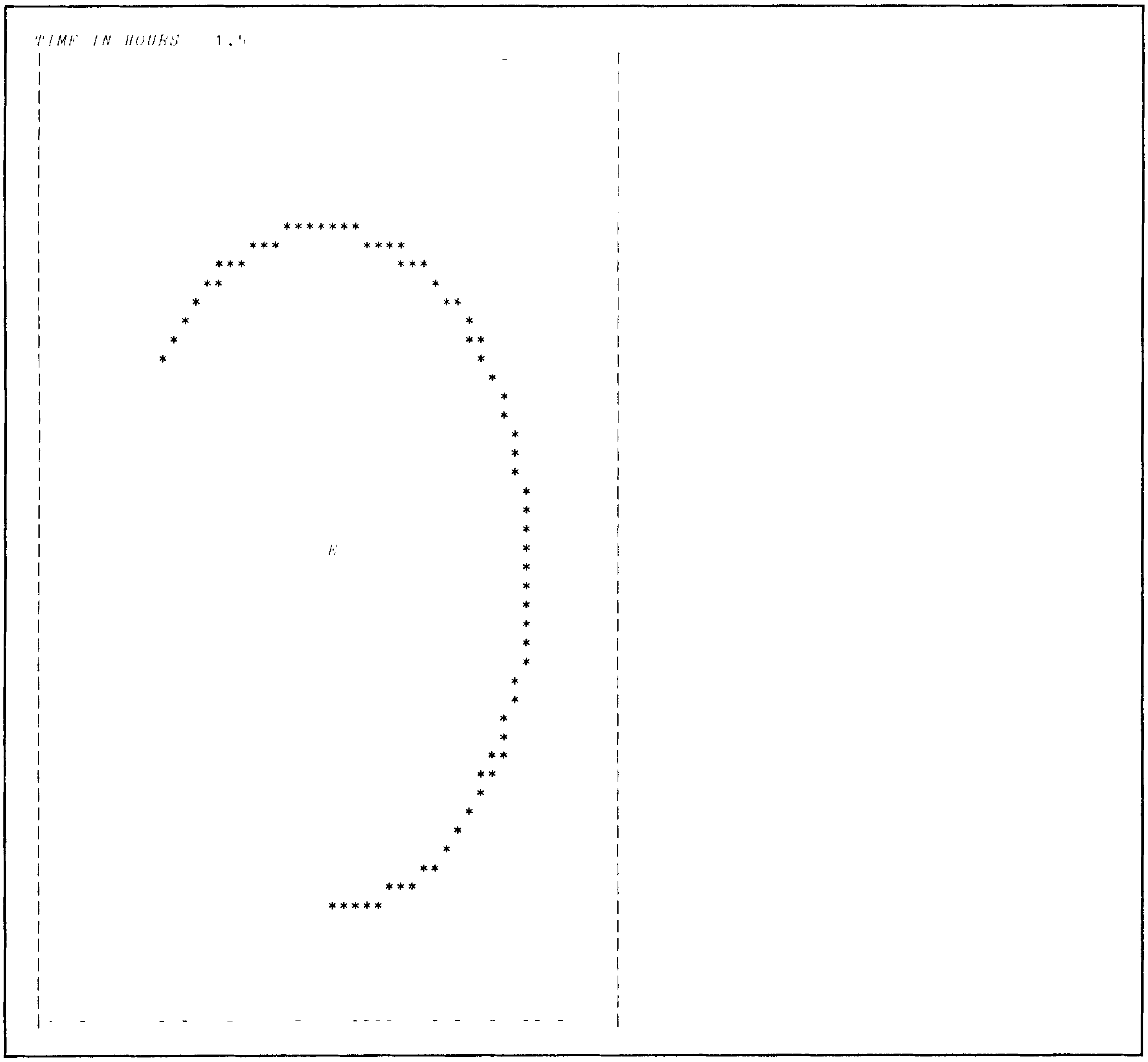
The program is given the masses of the bodies and their initial positions and velocities. The units used are seconds, meters, and kilograms. This is a simplified version with only two bodies and minimal computer graphics.

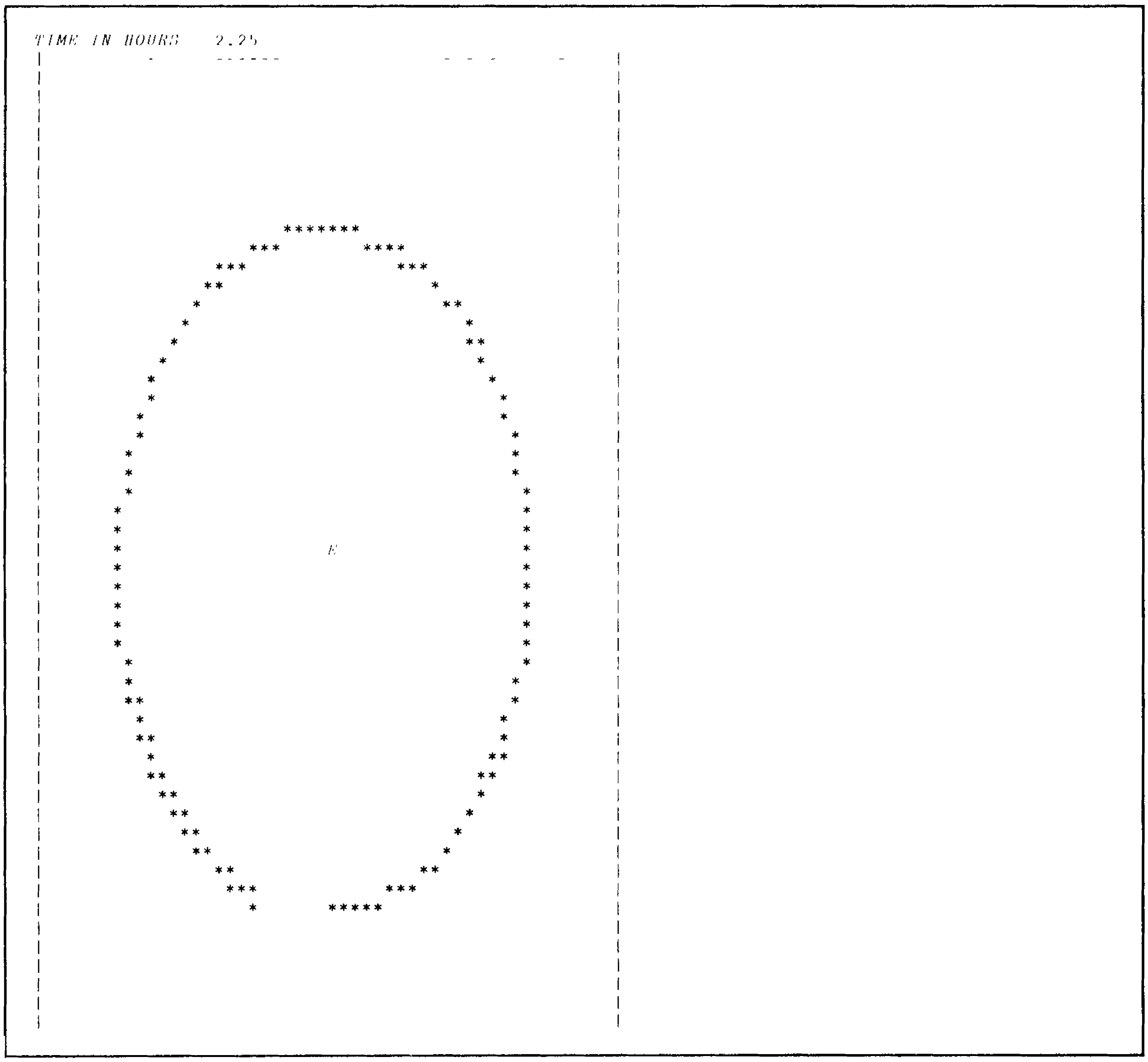
More precisely, we simulate an artificial satellite orbiting around the earth. Here are the initial conditions. The masses of earth and of the satellite are 6×10^{24} kilograms and 10 kilograms, respectively. The earth is initially at rest at the origin of coordinate system. The satellite is initially 10^7 meters from the center of the earth, which is about 2200 miles above the earth's surface, and is traveling at 6×10^3 meters per second (about 13400 miles per hour) perpendicular to the radius vector connecting it to the earth's center.

We use a time step of sixty seconds in the calculation, and draw a motion picture frame every fifteen time steps, i.e., every quarter hour of simulated time. Altogether, we draw twelve pictures of the orbit. Thus the total simulated time is three hours.

We do not have to worry about how to draw a picture of a three dimensional situation, because we have set things up in such a manner that the last coordinate of the position of the earth and the satellite is identically zero. Each picture of the trajectory is a 50 by 50 array of pixels (picture elements), in this case single characters. Each pixel represents a square that is 500 kilometers by 500 kilometers. The earth is represented by the letter "E," and the satellite is represented by an asterisk "*."


TIME IN HOURS 0.75
E


TIME IN HOURS 1.5
E


TIME IN HOURS 2.25
E

2. The Electromagnetic Field: Maxwell's Equations

It may be preferable to build up to the 4-vector potential version of Maxwell's equations that we present here, by first considering a program for the traditional form of Maxwell's equations based directly on E and B.

Readings

- Einstein & Infield, Chapters 2 & 3, "The Decline of the Mechanical View," & "Field, Relativity", for the concepts
- Feynman, Leighton & Sands, for the formulas

Additional References

- Potter, on centered integration
- Moriyasu, on Maxwell's equations in gauge theory

Maxwell—4-Vector Potential Vacuum Field Equations

```
      )LOAD MAXWELL
SAVED 1985-02-14 10.39.15 (GMT 5) 2727K(2723K)

      ∇MAXWELL[⎕]∇
[ 0]   MAXWELL
[ 1]   ⎕IO←0
[ 2]   O←N←20
[ 3]   M←L←1
[ 4]   DELTA←1
[ 5]   A←O N M L 4⍴0
[ 6]   A[0;;;;2]← (÷○2÷N)×2○○2×(⍳N)÷N
[ 7]   A[1;;;;2]←-(÷○2÷N)×2○○2×((-DELTA)+⍳N)÷N
[ 8]   T←1
[ 9]  LOOP:
[10]   X←(1⌽[0]A[T;;;;])+(1⌽[1]A[T;;;;])+(1⌽[2]A[T;;;;])
[11]   Y←(¯1⌽[0]A[T;;;;])+(¯1⌽[1]A[T;;;;])+(¯1⌽[2]A[T;;;;])
[12]   A[T+1;;;;]←X+Y-A[T-1;;;;]+4×A[T;;;;]
[13]   →(O>1+T←T+1)/LOOP
[14]   DA←O N M L 4 4⍴0
[15]   DA[;;;;;0]←((1⌽[0]A)-(¯1⌽[0]A))÷2×DELTA
[16]   DA[;;;;;1]←-((1⌽[1]A)-(¯1⌽[1]A))÷2×DELTA
[17]   DA[;;;;;2]←-((1⌽[2]A)-(¯1⌽[2]A))÷2×DELTA
[18]   DA[;;;;;3]←-((1⌽[3]A)-(¯1⌽[3]A))÷2×DELTA
[19]   'LORENTZ CONDITION: MAX |DIV| = 0?'
[20]   ⌈/,|+/0 1 2 3 4 4⍉DA
[21]   F←(0 1 2 3 5 4⍉DA)-DA
[22]   T←0
[23]  LOOP2:
[24]   DRAW
[25]   →(O>T←T+1)/LOOP2

      ∇DRAW[⎕]∇
[0]  DRAW
[1]  'Ex' SHOW F[T;;0;0;1;0]
[2]  'Ey' SHOW F[T;;0;0;2;0]
[3]  'Ez' SHOW F[T;;0;0;3;0]
[4]  'Bx' SHOW F[T;;0;0;3;2]
[5]  'By' SHOW F[T;;0;0;1;3]
[6]  'Bz' SHOW F[T;;0;0;2;1]

      ∇SHOW[⎕]∇
[0]  NAME SHOW F
[1]  →(∧/0=F)/0
[2]  ' '
[3]  NAME,' AT TIME = ',⍕T×DELTA
[4]  FRAME(-⌊26+25×F)⌽((⍴F),52)⍴'*',51⍴' '

      ∇FRAME[⎕]∇
[0]  FRAME PIC
[1]  '-',[0]('|',' ',' ',(⍕N 1⍴⍳N),' ',' ','|',PIC,'|'),[0]'-'
```

This program presents the modern relativistic version of Maxwell's equations in the form that is used in quantum mechanics, and which inspired gauge theory. The electrical and magnetic fields E and B play a subordinate role; the principal actor is the 4-vector potential A_u consisting of the scalar potential ϕ and the vector potential A.

Let's start by stating the Maxwell's equations in terms of the scalar potential ϕ and the vector potential A. Then we will restate this in terms of the 4-vector potential A_u.

Here are Maxwell's vacuum field equations in terms of ϕ and A.

$$E = -\nabla\phi - \frac{\partial A}{\partial t}$$

$$B = \nabla \times A$$

$$\nabla^2\phi - \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = 0$$

$$\nabla^2 A - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} = 0$$

$$\nabla \bullet A - \frac{1}{c^2}\frac{\partial\phi}{\partial t} = 0$$

Here is a more explicit version of these equations, written in terms of components:

$$E = (E_x, E_y, E_z) = -\left(\frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \frac{\partial\phi}{\partial z}\right) - \left(\frac{\partial A_x}{\partial t}, \frac{\partial A_y}{\partial t}, \frac{\partial A_z}{\partial t}\right)$$

Thus

$$E = -\left(\frac{\partial\phi}{\partial x} + \frac{\partial A_x}{\partial t}, \frac{\partial\phi}{\partial y} + \frac{\partial A_y}{\partial t}, \frac{\partial\phi}{\partial z} + \frac{\partial A_z}{\partial t}\right)$$

As for B,

$$B = (B_x, B_y, B_z) = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}, \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}, \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)$$

Then we have four very similar equations giving the time evolution of ϕ and the components of A:

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = 0$$

$$\frac{\partial^2 A_x}{\partial x^2} + \frac{\partial^2 A_x}{\partial y^2} + \frac{\partial^2 A_x}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2 A_x}{\partial t^2} = 0$$

$$\frac{\partial^2 A_y}{\partial x^2} + \frac{\partial^2 A_y}{\partial y^2} + \frac{\partial^2 A_y}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2 A_y}{\partial t^2} = 0$$

$$\frac{\partial^2 A_z}{\partial x^2} + \frac{\partial^2 A_z}{\partial y^2} + \frac{\partial^2 A_z}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2 A_z}{\partial t^2} = 0$$

Finally, here is the Lorentz gauge condition again:

$$\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} - \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0$$

Now, let's reformulate this in 4-vector notation, and let's take the speed of light to be unity $c = 1$. The 4-vector A_u is defined as follows:

$$A_u = (A_0, A_1, A_2, A_3) = (\phi, A) = (\phi, A_x, A_y, A_z)$$

We also need to introduce the partial differentiation operator ∂_u :

$$\partial_u = \left(\frac{\partial}{\partial t}, -\frac{\partial}{\partial x}, -\frac{\partial}{\partial y}, -\frac{\partial}{\partial z}\right)$$

Similarly, the D'Alembertian operator $\Box$ is

$$\Box = \left(\frac{\partial^2}{\partial t^2}, -\nabla^2\right) = \left(\frac{\partial^2}{\partial t^2}, -\frac{\partial^2}{\partial x^2}, -\frac{\partial^2}{\partial y^2}, -\frac{\partial^2}{\partial z^2}\right)$$

From A_u is obtained the antisymmetric tensor F_{uv} (i.e., $F_{uv} = -F_{vu}$), whose six independent components are the components of E and B.

$$F_{uv} = \partial_u A_v - \partial_v A_u$$

Then E and B are determined as follows:

$$F_{uv} = \begin{bmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & -B_z & B_y \\ E_y & B_z & 0 & -B_x \\ E_z & -B_y & B_x & 0 \end{bmatrix}$$

And the field equations become

$$\Box A_u = 0$$

while the Lorentz gauge condition is

$$\partial_0 A_0 + \partial_1 A_1 + \partial_2 A_2 + \partial_3 A_3 = 0$$

Now we discuss the formulation as difference equations. First of all, we make the important decision that $\Delta t = \Delta x = \Delta y = \Delta z = \Delta$. Next, we replace first and second order partial derivatives by differences as follows:

$$\frac{\partial f}{\partial x} = \frac{f(x+\Delta) - f(x-\Delta)}{2\,\Delta}$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{\left[\dfrac{f(x+\Delta) - f(x)}{\Delta}\right] - \left[\dfrac{f(x) - f(x-\Delta)}{\Delta}\right]}{\Delta} = \frac{f(x+\Delta) - 2\,f(x) + f(x-\Delta)}{\Delta^2}$$

Then the crucial piece of reasoning is as follows.

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} = 0$$

(recall $c = 1$) can be expressed as

$$\frac{\psi(t+\Delta) - 2\psi + \psi(t-\Delta)}{\Delta^2} =$$
$$\frac{\psi(x+\Delta) - 2\psi + \psi(x-\Delta)}{\Delta^2} +$$
$$\frac{\psi(y+\Delta) - 2\psi + \psi(y-\Delta)}{\Delta^2} +$$
$$\frac{\psi(z+\Delta) - 2\psi + \psi(z-\Delta)}{\Delta^2}$$

This difference equation is space and time centered and therefore highly accurate. Multiplying through by Δ^2, and rearranging things slightly, we get

$$\begin{aligned}\psi(t+\Delta) = &- 4\psi - \psi(t-\Delta)\\ &+ \psi(x+\Delta) + \psi(y+\Delta) + \psi(z+\Delta)\\ &+ \psi(x-\Delta) + \psi(y-\Delta) + \psi(z-\Delta)\end{aligned}$$

This yields a "leapfrog" method, i.e., from $\psi(t)$ and $\psi(t+1)$, we calculate $\psi(t+2)$, then from $\psi(t+1)$ and $\psi(t+2)$, we calculate $\psi(t+3)$, etc. This technique is simultaneously used on each component $\psi = A_u$ of the 4-vector potential, since these evolve independently.

Now we consider a solution to these equations which is a plane wave propagating along the x axis. We take

$$A_u = [0,\ 0,\ f(x-t),\ 0]$$

so that

$$E = -\left[0,\ \frac{\partial}{\partial t} f(x-t),\ 0\right] = -[0,\ -f'(x-t),\ 0] = [0,\ f'(x-t),\ 0]$$

and

$$B = \left[0,\ 0,\ \frac{\partial}{\partial x} f(x-t)\right] = [0,\ 0,\ f'(x-t)]$$

Thus E and B are always of equal magnitude and perpendicular to each other and to the direction of propagation. With this choice of A_u the field equations simplify greatly, since

$$A_0 = A_1 = A_3 = 0$$

and

$$\frac{\partial A_2}{\partial y} = \frac{\partial A_2}{\partial z} = 0$$

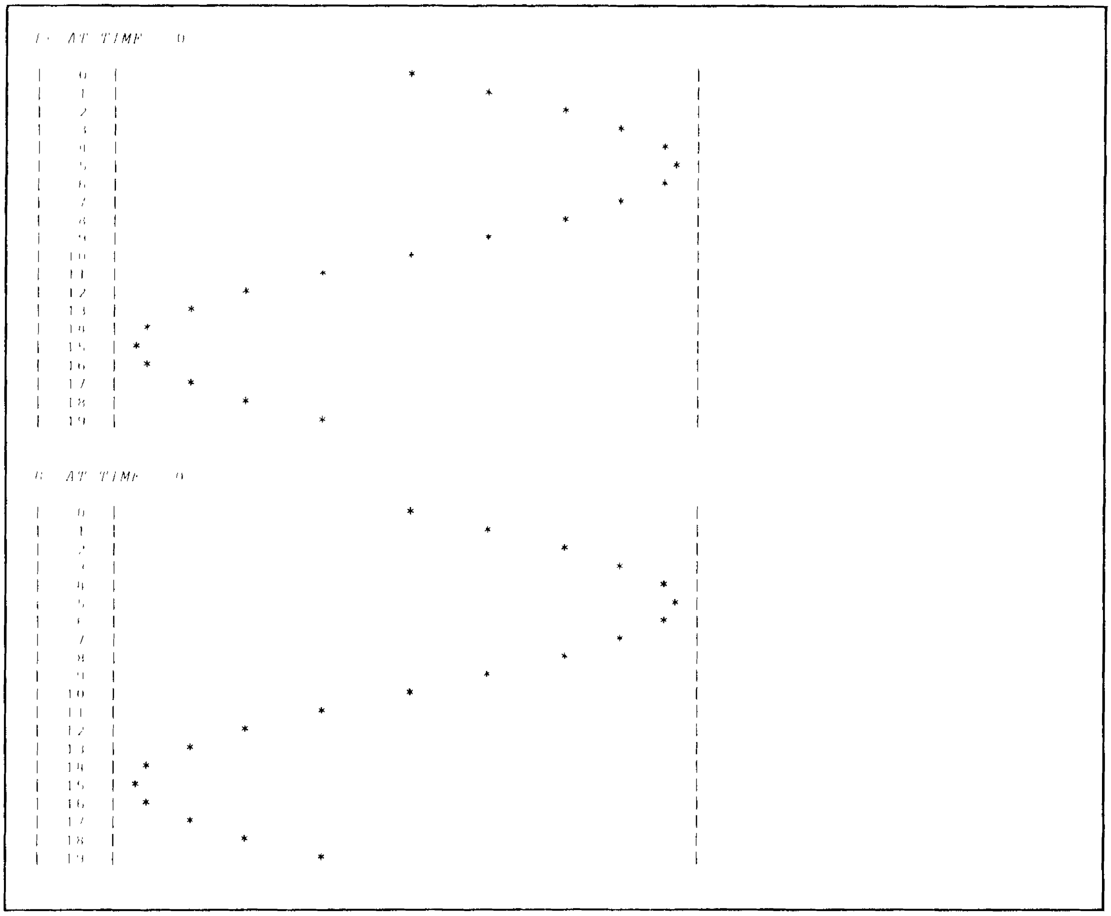
Thus to verify that Maxwell's equations are satisfied, it is sufficient to note that

$$\square A_2 = \frac{\partial^2}{\partial t^2} A_2 - \frac{\partial^2}{\partial x^2} A_2 = (--f''(x-t)) - f''(x-t) = 0$$

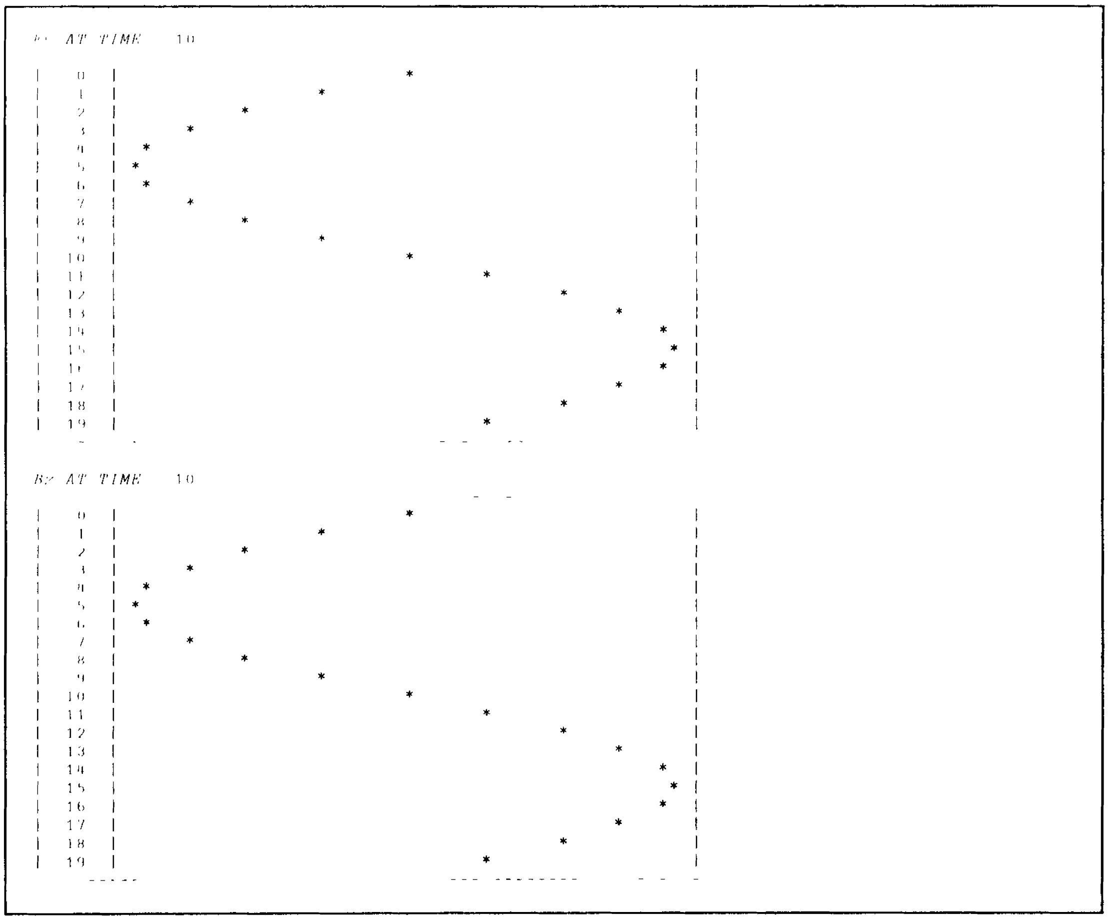
and

$$\partial_u A_u = \partial_2 A_2 = -\frac{\partial}{\partial y} f(x-t) = 0$$

In *Maxwell*, we consider for 20 time steps a world with periodic boundary conditions that is $20 \times 1 \times 1$, which essentially reduces us to the case of a one-dimensional field. And we take $f(x) = -(20/2\pi)\cos(2\pi x/20)$, so that $f' = \sin(2\pi x/20)$.



In this picture and the one on the next page, the field strength -1 is flush left, 0 is in the middle, and $+1$ is flush right.


AT TIME 10
AT TIME 10

3. Curved Space-Time: Einstein's Field Equations for Gravity

Our first program, *Einst*, repeats the orbit calculation that was done in the program *Newton* in Chapter 1, and fortunately the result of the general relativity calculation is essentially the same as the one we obtained before. The metric used in this program is an approximate one, and is an easy consequence of special relativity and the principle of equivalence applied to the gravitational field experienced on a rotating disk. Paradoxically, if this program is improved to use the Schwarzschild metric, it gives much worse results. The reason better physics gives worse numbers, is that the mathematical method employed works better in rectangular coordinates than in polar coordinates.

Readings

- Einstein & Infield, Chapter 3, "Field, Relativity."
- Einstein *Relativity*, for the merry-go-round
- Skinner, for the meaning of Γ and R
- Einstein *The Meaning of Relativity*, for the formulas for Γ and R and the fact that the gravitational time dilation metric gives Newton's equations of motion
- Eddington, for the meaning of curvature
- Penrose, for a geometrical statement of the field equations
- Harris, for a discussion of different approximations to the Schwarzschild metric
- Unsöld, for a summary of relativistic cosmology

Additional References

- Rindler

Einst—Geodesics in Rectangular Coordinates

```
        )LOAD EINST
SAVED 1985-01-08 19.04.43 (GMT-5) 2727K(2695K)

        ∇EINST[⎕]∇
[ 0]     EINST
[ 1]     ⎕IO←1
[ 2]     ORBIT←50 50⍴' '
[ 3]     E←1000
[ 4]     DELT←60
[ 5]     C←3E8
[ 6]     DX←(X←1E7,(DELT×6E3),0,(DELT×C))  (1E7,0,0,0)
[ 7]     STEP←2
[ 8]    LOOP:
[ 9]     DRAW X←X+DX←DX-((GAMMA X)+.×DX)+.×DX
[10]     →((12×15)≥STEP←STEP+1)/LOOP

        ∇DRAW[⎕]∇
[0]     DRAW X
[1]     ORBIT[25+0;25+0]←'E'
[2]     ORBIT[25+⌊X[1]÷5E5;25+⌊X[2]÷5E5]←'*'
[3]     →(0≠15|STEP)/0
[4]     ' '
[5]     'TIME IN HOURS - ',⍕X[4]÷60×60×C
[6]     FRAME ORBIT

        ∇G[⎕]∇
[0]     Z←G X
[1]     Z←4 4⍴0
[2]     (1 1⍉Z)←(¯1 ¯1 ¯1),1-.0088÷(+/3↑X*2)*.5

        ∇DGDX[⎕]∇
[0]     Z←DGDX X
[1]     Z←⊃[1 2]((G¨⊂[2]X+Z)-(G¨⊂[2](X←4 4⍴X)-Z←E×(⍳4)∘.=⍳4))÷2×E

        ∇GAMMA[⎕]∇
[0]     Z←GAMMA X
[1]     Z←.5×(⌹G X)+.×(2 1 3⍉Z)+(3 1 2⍉Z)-(2 3 1⍉Z←DGDX X)

        ∇FRAME[⎕]∇
[0]     FRAME PIC
[1]     '|',('-',[1]PIC,[1]'-'),'|'
```

The program *Einst* does the following. Given two close initial points in space-time, it calculates the motion of a small test particle according to the weak field nonrelativistic motion metric resulting from the principle of equivalence. This is given by the geodesic passing through those points.

More precisely, we calculate the trajectory of an artificial satellite orbiting the earth. The mass of the earth is 6×10^{24} kilograms, which is .0088 meters in units in which $G = c = 1$, and the earth is at rest at the origin of coordinate system. The satellite is initially 10^7 meters from the center of the earth, which is about 2200 miles above the earth's surface, and is traveling at 6×10^3 meters per second (about 13400 miles per hour) perpendicular to the radius vector connecting it to the earth's center. These initial conditions give us the first point on the trajectory. In order to determine a geodesic passing through it, we need a second point on the trajectory. We get this point by estimating where the artificial satellite will be sixty seconds later, assuming that for the first minute the gravitational effect due to the earth is negligible and the satellite travels in a straight line.

This gives us a sixty second time step in the calculation, and we draw a motion picture frame every fifteen time steps, i.e., every quarter hour of simulated time. Altogether, we draw twelve pictures of the orbit. Thus the total simulated time is three hours.

The first subroutine, *DRAW*, draws a picture of the geodesic trajectory. We do not have to worry about how to draw a picture of a three dimensional situation, because we have set things up in such a manner that the z coordinate of the position of the earth and the satellite is identically zero. Each picture of the trajectory is a 50 by 50 array of pixels (picture elements), in this case single characters. Each pixel represents a square that is 500 kilometers by 500 kilometers. The earth is represented by the letter "E," and the satellite is represented by an asterisk "*."

Below we use Einstein's summation convention: any term with repeated indices denotes the sum over all values of this index (1, 2, 3, and 4).

The next subroutine, G, calculates the 4×4 matrix consisting of the coefficients of $dx_i\, dx_j$ in the fundamental metric form, which gives the distance ds between two infinitesimally close points in terms of the differences between their coordinates:

$$ds^2 = g_{ij}\, dx_i\, dx_j$$

These sixteen values of g_{ij} as a function of x_1, x_2, x_3 and x_4 define a space-time and determine all its geometrical properties. g must be a symmetrical function of i and j. Given a point X in space-time, G produces the 4×4 matrix of the g_{ij} at that point. For convenience in defining the particular metric that we use, let

$$\begin{cases} x_1 = x \\ x_2 = y \\ x_3 = z \\ x_4 = t \end{cases}$$

Here is the gravitational time dilation metric for a point mass:

$$ds^2 = \left[1 - \frac{2m}{\sqrt{x^2 + y^2 + z^2}} \right] dt^2 - \left(dx^2 + dy^2 + dz^2\right)$$

Here x, y, z are the usual rectangular coordinates measured in meters, and the mass m and time t are measured in units in which $G = c = 1$.

Let us be more explicit. Since light travels 3×10^8 meters per second, our unit of distance is meters, and our unit of time is such that the speed of light is unity, it follows that one second is equal to 3×10^8 of these time units. And our unit of mass is the normal one multiplied by the gravitational coupling constant G and divided by the speed of light squared. In these units the mass of the earth is $(6 \times 10^{24})(.667 \times 10^{-10})/(3 \times 10^8)^2 = .44$ centimeters, and thus the radius of the event horizon of the earth, i.e., the Schwarzschild radius of the earth, is $2m = .0088$ meters.

The next subroutine, *DGDX*, calculates the $4 \times 4 \times 4$ matrix consisting of the partial derivatives of the g_{ij} with respect to the x_k at a point X in space-time.

$$\frac{\partial g_{ij}}{\partial x_k} = g_{ij,\,k}$$

The next subroutine, *GAMMA*, calculates the connection Γ at a point X in space-time, which is also known as the Christoffel symbol of the second kind. This consists of a 4×4×4 matrix used to calculate the result of an infinitesimal parallel displacement of a vector from the point X:

$$\begin{aligned}\Gamma^s_{uv} &= \frac{1}{2} g^{sa} \left(\frac{\partial g_{ua}}{\partial x_v} + \frac{\partial g_{va}}{\partial x_u} - \frac{\partial g_{uv}}{\partial x_a} \right) \\ &= \frac{1}{2} g^{sa} \left(g_{ua,\,v} + g_{va,\,u} - g_{uv,\,a} \right)\end{aligned}$$

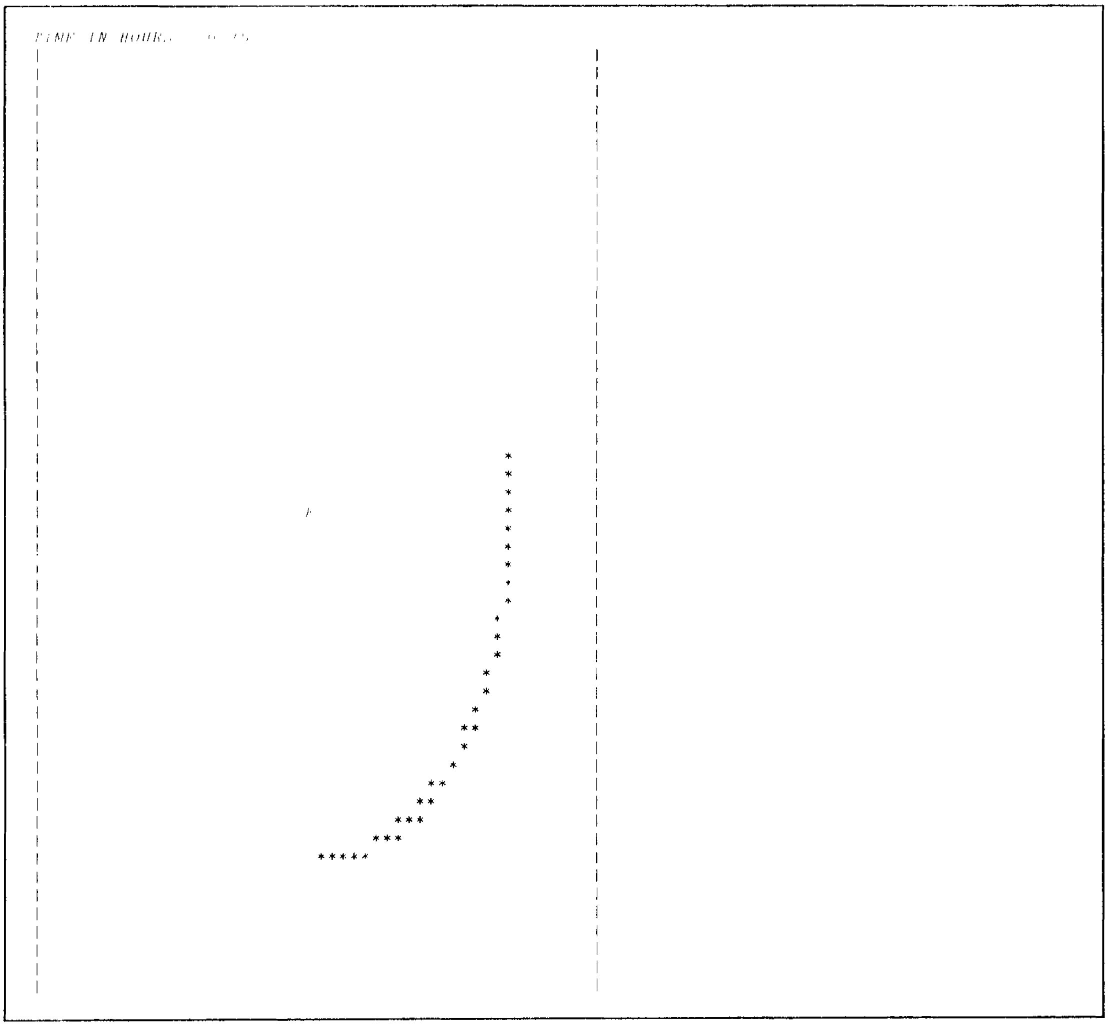
Here g written with superscripts rather than subscripts denotes the metric inverse, a 4×4 matrix which is defined as follows

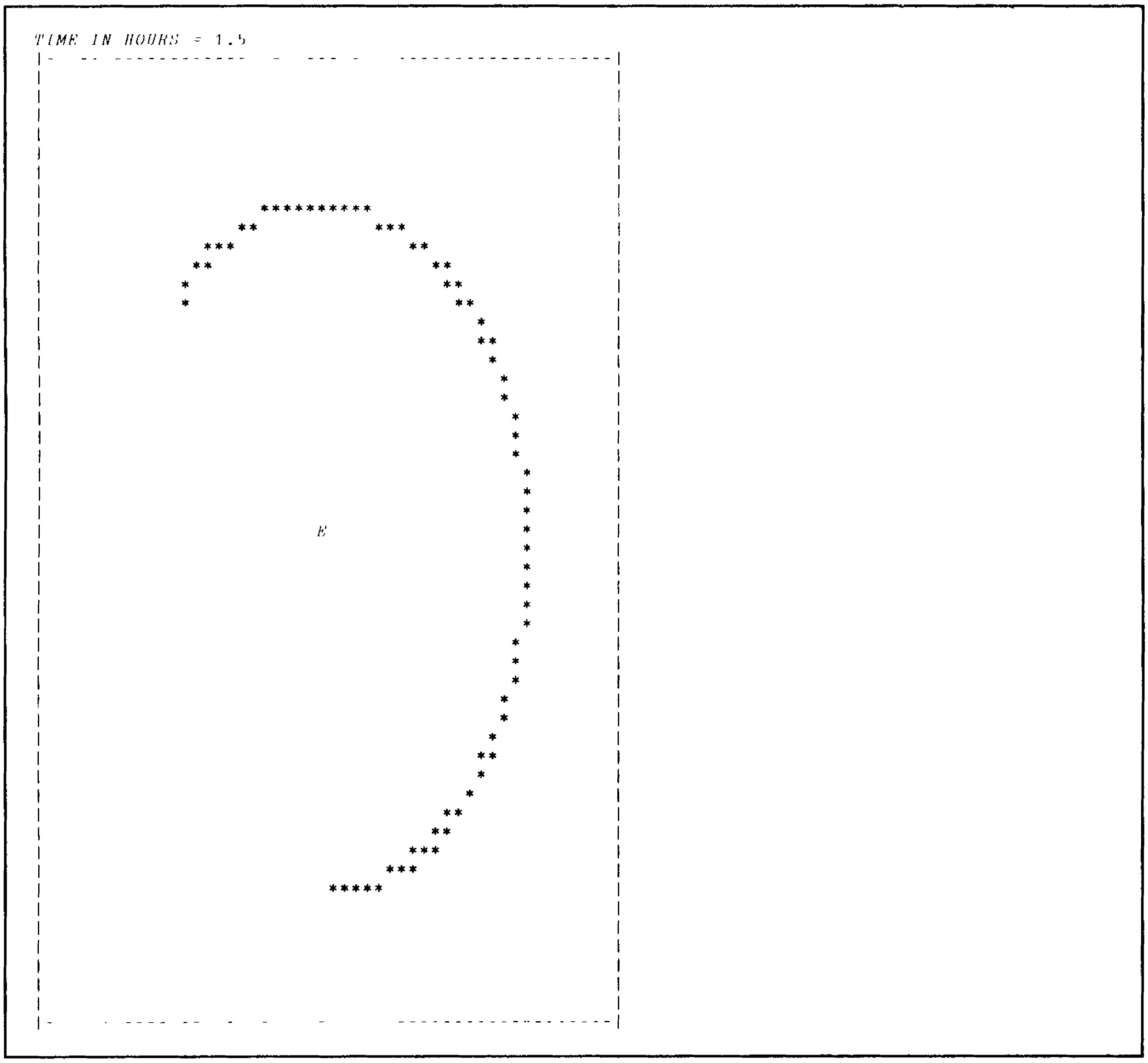
$$g_{ik}\, g^{kj} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

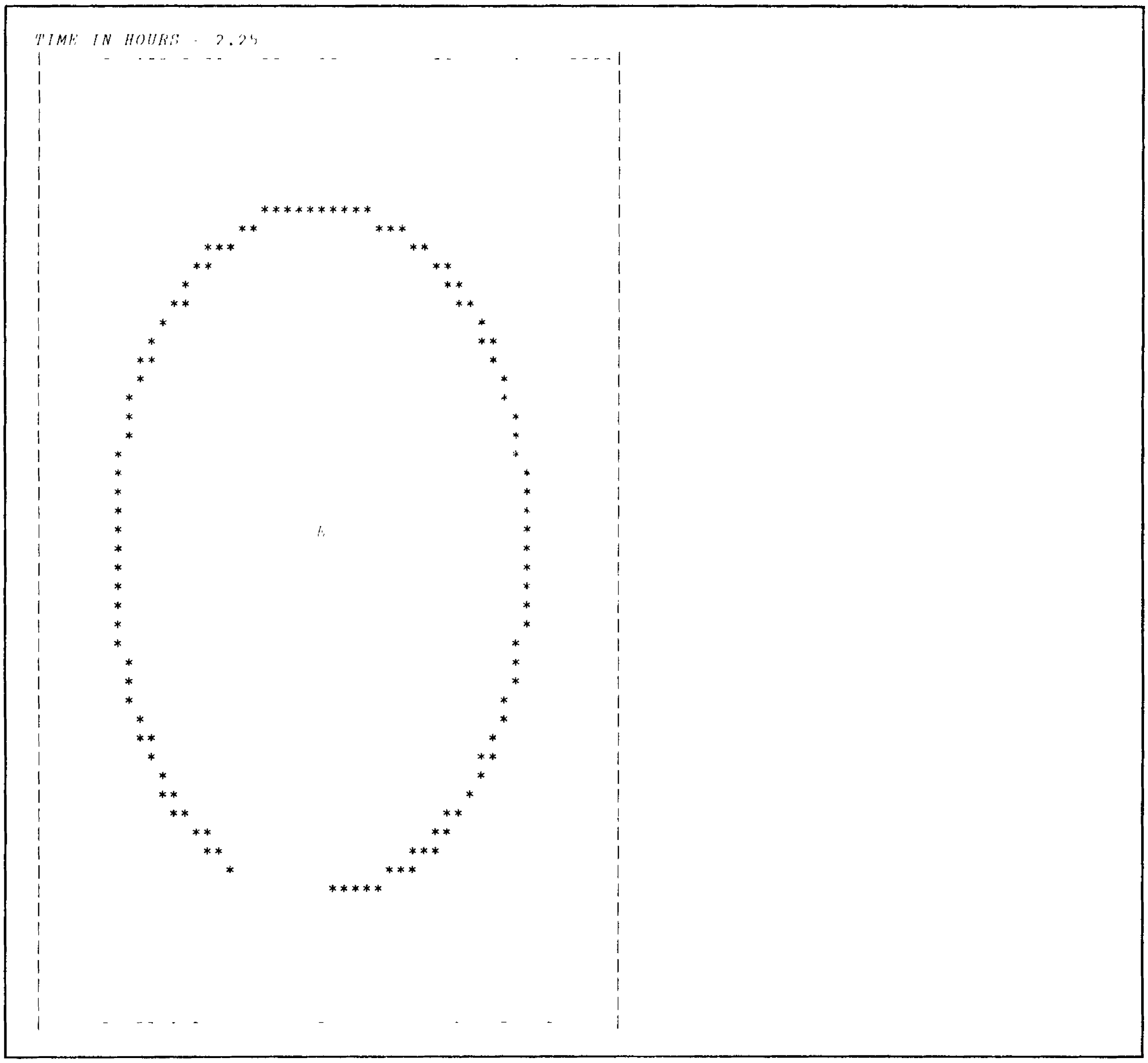
and which is calculated using the APL matrix inverse function ⌹.

Finally here is the equation for a geodesic:

$$\frac{d^2 x_u}{ds^2} + \Gamma^u_{ab} \frac{dx_a}{ds} \frac{dx_b}{ds} = 0$$




TIME IN HOURS = 1.5
E


TIME IN HOURS - 2.25

Einst2—Numerical Verification of the Curvature near a Black Hole

```
      )LOAD EINST2
SAVED 1985-01-08 19.04.29 (GMT-5) 2727K(2695K)

      ∇EINST2[⎕]∇
[ 0]   EINST2
[ 1]   ⎕IO←1
[ 2]   'EPSILON = ',⍕E←.0001
[ 3]   'X = ',⍕X←2 1 1 0
[ 4]   ' '
[ 5]   'RIEMANN CURVATURE TENSOR ='
[ 6]   ⎕←R←R4 X
[ 7]   ' '
[ 8]   'WILL SUM:'
[ 9]   3 1 2 3⍉R
[10]   ' '
[11]   'RICCI TENSOR ='
[12]   +/3 1 2 3⍉R

      ∇G[⎕]∇
[0]   Z←G X
[1]   Z←4 4⍴0
[2]   (1 1⍉Z)←(-÷1-÷X[1]),(-X[1]*2),(-(X[1]×1○X[2])*2),1-÷X[1]

      ∇G2[⎕]∇
[0]   Z←G2 X
[1]   (1 1⍉Z)←÷1 1⍉Z←G X

      ∇DGDX[⎕]∇
[0]   Z←DGDX X
[1]   Z←⊃[1 2]((G¨⊂[2]X+Z)-(G¨⊂[2](X←4 4⍴X)-Z←E×(⍳4)∘.=⍳4))÷2×E

      ∇GAMMA[⎕]∇
[0]   Z←GAMMA X
[1]   Z←.5×(G2 X)+.×(2 1 3⍉Z)+(3 1 2⍉Z)-(2 3 1⍉Z←DGDX X)

      ∇DGAMMADX[⎕]∇
[0]   Z←DGAMMADX X
[1]   Z←⊃[1 2 3]((GAMMA¨⊂[2]X+Z)-(GAMMA¨⊂[2](X←4 4⍴X)-Z←E×(⍳4)∘.=⍳4))÷2×E

      ∇R4[⎕]∇
[0]   Z←R4 X
[1]   Z←(1 3 2⍉Z)+.×Z←GAMMA X
[2]   Z←(-Z)+(1 2 4 3⍉Z←DGAMMADX X)+(1 3 2 4⍉Z)-(1 4 2 3⍉Z)
```

The program *Einst2* checks the Schwarzschild solution of the vacuum field equations of general relativity numerically at a single point of space-time. This involves calculating the Riemann curvature tensor at that point, and checking that various components sum to zero. More precisely, we check Einstein's field equations for gravity two meters from the center of a black hole with a Schwarzschild radius of one meter.

Below we use Einstein's summation convention: any term with repeated indices denotes the sum over all values of this index (1, 2, 3, and 4).

The first subroutine, G, calculates the 4×4 matrix consisting of the coefficients of $dx_i\,dx_j$ in the fundamental metric form, which gives the distance ds between two infinitesimally close points in terms of the differences between their coordinates:

$$ds^2 = g_{ij}\,dx_i\,dx_j$$

These sixteen values of g_{ij} as a function of x_1, x_2, x_3 and x_4 define a space-time and determine all its geometrical properties. g must be a symmetrical function of i and j. Given a point X in space-time, G produces the 4×4 matrix of the g_{ij} at that point. For convenience in defining the particular metric that we use, let

$$\begin{cases} x_1 = r \\ x_2 = \theta \\ x_3 = \phi \\ x_4 = t \end{cases}$$

Here is the Schwarzschild metric for a point mass:

$$ds^2 = \left(1 - \frac{2m}{r}\right)dt^2 - \left[\frac{dr^2}{\left(1 - \frac{2m}{r}\right)} + r^2\left(\sin^2\theta\,d\phi^2 + d\theta^2\right)\right]$$

Here r, θ, ϕ are the usual spherical polar coordinates, measuring, respectively, distance from the origin in meters, inclination from the z axis in radians, and angle around the z axis in radians. And the mass m and time t are measured in units in which $G = c = 1$.

The next subroutine, $G2$, calculates the metric inverse, which is a diagonal 4×4 matrix defined as follows:

$$g_{ik}\,g^{kj} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

In *Einst* we simply calculated the metric inverse by using the APL matrix inverse function ⌹. In *Einst2* we take advantage of the fact that the Schwarzschild metric is diagonal to get a more accurate metric inverse by simply replacing each element in the diagonal of the metric by its reciprocal. This additional accuracy was not needed in *Einst*.

The next subroutine, $DGDX$, calculates the 4×4×4 matrix consisting of the partial derivatives of the g_{ij} with respect to the x_k:

$$\frac{\partial g_{ij}}{\partial x_k} = g_{ij,\,k}$$

The next subroutine, $GAMMA$, calculates the connection Γ at a point X in space-time, which is also known as the Christoffel symbol of the second kind. This is a 4×4×4 matrix used to calculate the result of an infinitesimal parallel displacement of a vector from the point X:

$$\Gamma^{s}_{uv} = \frac{1}{2} g^{sa} \left(\frac{\partial g_{ua}}{\partial x_v} + \frac{\partial g_{va}}{\partial x_u} - \frac{\partial g_{uv}}{\partial x_a} \right)$$
$$= \frac{1}{2} g^{sa} \left(g_{ua,\,v} + g_{va,\,u} - g_{uv,\,a} \right)$$

The next subroutine, *DGAMMADX*, calculates the 4×4×4×4 matrix consisting of the partial derivatives of the connection components at the point X:

$$\frac{\partial \Gamma^{i}_{jk}}{\partial x_l} = \Gamma^{i}_{jk,\,l}$$

The next subroutine, *R4*, produces the Riemann curvature tensor, which is a 4×4×4×4 matrix used to calculate the change in a vector at X after parallel displacement around an infinitesimal parallelogram:

$$R^{u}_{sab} = -\frac{\partial \Gamma^{u}_{sa}}{\partial x_b} + \frac{\partial \Gamma^{u}_{sb}}{\partial x_a} + \Gamma^{u}_{ra}\Gamma^{r}_{sb} - \Gamma^{u}_{rb}\Gamma^{r}_{sa}$$
$$= -\Gamma^{u}_{sa,\,b} + \Gamma^{u}_{sb,\,a} + \Gamma^{u}_{ra}\Gamma^{r}_{sb} - \Gamma^{u}_{rb}\Gamma^{r}_{sa}$$

A space-time is flat if and only if all the components of the Riemann curvature tensor are identically 0.

Finally, we calculate the Ricci tensor at the point X in space-time

$$R_{uv} = R^{a}_{uva}$$

which is a 4×4 matrix obtained from a 4×4×4 submatrix of the Riemann curvature tensor, and we check Einstein's vacuum field equations, i.e., that

$$R_{uv} = 0$$

```
WILL SUM:
0                0.1250000005     1.2500000498E-1   0.2500000046
0                0                1.9108240138E-1   0
0                0                0.0000000000E0    0
0                0                0.0000000000E0    0

0                0                1.9097137907E-9   0
0.249999972      0                5.0000000255E-1   0.2505000006
0                0                0.0000000000E0    0
0                0                0.0000000000E0    0

0                0                0.0000000000E0    0
0                0                0.0000000000E0    0
0.1770183589     0.3540936968     0.0000000000E0    0.17[illegible]
0                0                0.0000000000E0    0

0                0                0.0000000000E0    0
0                0                0.0000000000E0    0
0                0                0.0000000000E0    0
0.0625000021     0.0312500008     1.1250000083E-2   0

RICCI TENSOR
8.1001259877E-10   1.910824013[illegible]   1.6900000[illegible]E-6   0.0000000000E0
1.9097137790E-9    4.6683142956E-9          0.0000000000E0            0.0000000000E0
0.0000000000E0     0.0000000000E0           1.7088904[illegible]E-8   0.0000000000E0
0.0000000000E0     0.0000000000E0           0.0000000000E0            5.7848131167E-11
```

At the point of space-time under consideration, the components of the Ricci tensor are at least seven orders of magnitude smaller than the relevant components of the Riemann curvature tensor. This is therefore an excellent numerical verification that the Schwarzschild metric satisfies Einstein's vacuum field equations.

4. Quantum Probability Waves: Schrödinger's Equation in One Dimension

My original goal was to present here a working model of the hydrogen atom, but unfortunately it seems that much too much computation is needed and this is quite impractical. So instead of doing time evolution according to the Schrödinger equation in three dimensions, we work in one dimension.

Readings

- Einstein & Infield, Chapter 4, "Quanta."
- PSSC *Physics*, for the de Broglie wave length of a particle
- PSSC *Physics*, for the Bohr hydrogen atom
- Born, for a summary of the formalism of quantum mechanics
- Polkinghorne, for a summary of the formalism of quantum mechanics

Additional References

- Eisberg & Resnick
- Potter
- Gerald & Wheatley
- Goldberg, Schey & Schwartz

Schrod—One Dimensional Time Evolution

```
      )LOAD SCHROD
SAVED 1985-01-16 18.48.54 (GMT-5) 2727K(2663K)

      ∇SCHROD[⎕]∇
[ 0]   SCHROD
[ 1]   ⎕IO←0
[ 2]   I←0J1
[ 3]   HBAR←.1
[ 4]   MASS←1
[ 5]   DELX←1÷N←50
[ 6]   DELT←1÷STEPS←20×N
[ 7]   X←¯.5+(.5+⍳N)÷N
[ 8]   V←Nρ0 ⍝ TRY V←1000,((N-2)ρ0),1000 OR V←((⌊.8×N)ρ0),(N-⌊.8×N)ρ10
[ 9]   ALPHA←÷HBAR×I
[10]   BETA←-ALPHA×(HBAR*2)÷2×MASS×2×DELX*2
[11]   A←B←N Nρ0
[12]   A[;1]←A[;N-1]←-BETA
[13]   A[;0]←(÷DELT)+(2×BETA)-(ALPHA÷2)×V
[14]   B[;1]←B[;N-1]←BETA
[15]   B[;0]←(÷DELT)-(2×BETA)-(ALPHA÷2)×V
[16]   C←(⌹A←(-⍳N)⌽A)+.×B←(-⍳N)⌽B
[17]   X0←0
[18]   K0←30 ⍝ -15 GOES IN OPPOSITE DIRECTION AT HALF THE SPEED
[19]   SIGMA0←.05
[20]   PSI←(*K0×I×X)×(*-((X-X0)*2)÷(2×SIGMA0*2)) ⍝ TRY PSI←*(○2)×I×X
[21]   (TIME←0)DRAW PSI←PSI÷(+/|PSI*2)*.5
[22]   STEP←0
[23]  LOOP:→(STEPS<STEP←STEP+1)/0
[24]   PSI←C+.×PSI
[25]   TIME←TIME+DELT
[26]   →(0≠20|STEP)/LOOP
[27]   TIME DRAW PSI
[28]   →LOOP

      ∇DRAW[⎕]∇
[0]   TIME DRAW PSI
[1]   ' '
[2]   'PROBABILITY(POSITION) AT TIME - ',⍕TIME
[3]   'TOTAL PROBABILITY = ',⍕+/PROB←|PSI*2
[4]   FRAME(-⌈50×PROB÷⌈/PROB)⌽(N 51ρ'*',50ρ' ')
[5]   ' '
[6]   'PHASE(POSITION) AT TIME - ',⍕TIME
[7]   FRAME(-⌊22+I×1 1○⍟(PSI=0)+PSI)⌽(N 44ρ'#',43ρ' ')

      ∇FRAME[⎕]∇
[0]   FRAME PIC
[1]   PIC←(N 5ρ'|  V=' ),(⍕N 1ρV),' ',' ',(⍕N 1ρ⍳N),' ',' ','|',PIC,'|'
[2]   '-',[0]PIC,[0]'-'
```

Introduction

This program provides a one-dimensional working model of a quantum-mechanical particle moving in a potential. We use centered integration, which requires implicit solution of the difference equations, to get good numerical results. Boundary conditions are given for a Gaussian wave packet to propagate freely, and to scatter against a square barrier and inside an infinite well.

How does quantum mechanics describe the state of a particle by means of the complex valued wave function ψ, which possesses both a magnitude and a phase or angle at each point at which it is defined? The square of the magnitude of ψ at a point is proportional to the probability that the particle is there. And the rate at which the angle of ψ changes with position, i.e., the rate at which ψ rotates as position varies, is proportional to the momentum of the particle. (Rotation clockwise goes in one direction, counter clockwise moves in the opposite direction.) Also, the rate at which the angle of ψ changes with time, i.e., the rate at which ψ rotates as time varies, is proportional to the energy of the particle. (We have just stated the Schrödinger equation in words, in view of the relationship between momentum and energy given by $p^2/2m = (mv)^2/2m = mv^2/2$.) The Heisenberg uncertainty principle is reflected in the fact that if the velocity of a wave packet is known exactly, then ψ is a uniform rotation whose magnitude does not change as a function of position, so that the position is completely uncertain. Contrariwise, a spatially localized wave packet will contain a mixture of frequencies, that is, of momenta, and will spread with time.

Computational Technique

Here is Schrödinger's differential equation $\mathcal{E}\psi = \mathcal{H}\psi$ on a line:

$$\left(-\frac{\hbar}{i}\frac{\partial}{\partial t}\right)\psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\psi$$

I.e.,

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi\right)$$

This yields the following time and space centered finite difference equations:

$$\frac{\psi_{x,t+1} - \psi_{x,t}}{\Delta t} =$$

$$\frac{1}{i\hbar}\left[-\frac{\hbar^2}{2m}\left(\frac{\psi_{x+1,t+1} - 2\psi_{x,t+1} + \psi_{x-1,t+1}}{2(\Delta x)^2} + \frac{\psi_{x+1,t} - 2\psi_{x,t} + \psi_{x-1,t}}{2(\Delta x)^2}\right) + \frac{1}{2}\left(V_x\psi_{x,t+1} + V_x\psi_{x,t}\right)\right]$$

This can be expressed as the following system of linear equations:

$$\psi_{x+1,t+1}(-\beta) + \psi_{x,t+1}\left(\frac{1}{\Delta t} + 2\beta - \frac{\alpha}{2}V_x\right) + \psi_{x-1,t+1}(-\beta) =$$

$$\psi_{x+1,t}(\beta) + \psi_{x,t}\left(\frac{1}{\Delta t} - 2\beta + \frac{\alpha}{2}V_x\right) + \psi_{x-1,t}(\beta)$$

where

$$\alpha = \frac{1}{i\hbar} \qquad \beta = \alpha\left(-\frac{\hbar^2}{2m}\right)\frac{1}{2(\Delta x)^2}$$

Thus we are led to a matrix formulation of the time evolution of the wave function ψ according to the Schrödinger equation: the matrix A times the column vector of ψ values at time $t + 1$ is equal to the matrix B times the column vector of ψ values at time t:

$$A \begin{bmatrix} \psi_{0,\,t+1} \\ \vdots \\ \psi_{N-1,\,t+1} \end{bmatrix} = B \begin{bmatrix} \psi_{0,\,t} \\ \vdots \\ \psi_{N-1,\,t} \end{bmatrix}$$

where matrix A has the following element at row i and column j:

$$\begin{cases} -\beta & \text{if } j = i + 1 \text{ or } i - 1 \\ \dfrac{1}{\Delta t} + 2\,\beta - \dfrac{\alpha}{2} V_i & \text{if } j = i \end{cases}$$

and matrix B has the following element at row i and column j:

$$\begin{cases} \beta & \text{if } j = i + 1 \text{ or } i - 1 \\ \dfrac{1}{\Delta t} - 2\,\beta + \dfrac{\alpha}{2} V_i & \text{if } j = i \end{cases}$$

Thus the column vector of ψ values at time $t + 1$ is equal to (the inverse of matrix A) times matrix B times the column vector of ψ values at time t:

$$\begin{bmatrix} \psi_{0,\,t+1} \\ \vdots \\ \psi_{N-1,\,t+1} \end{bmatrix} = A^{-1} B \begin{bmatrix} \psi_{0,\,t} \\ \vdots \\ \psi_{N-1,\,t} \end{bmatrix}$$

The program *Schrod* deals with a one dimensional "world" one meter long in which the position x goes from $-.5$ to $.5$ with periodic boundary conditions. We simulate this world from $t = 0$ to $t = 1$, i.e., for one second. We take $\Delta x = 1/50$ and $\Delta t = 1/(20 \times 50)$, but we only draw a picture of the wave function ψ every 20 time steps. Thus the one meter space is divided into 50 cells, and the one second time is divided into a motion picture with 50 frames. Each frame is in two parts, a drawing of the probability as a function of position, and a drawing of the phase as a function of position, in which the positions are given as cell #'s going from 1 to 50. Along with each frame, we print the total probability, and this value, which should always be exactly unity, is indeed very accurately conserved.

Experiment 1—A Momentum Eigenstate

V is identically zero, that is to say, there is no potential and we are looking at free propagation.

Here is the formula for the initial wave function, which is included in *Schrod* as a comment (see line [20]):

$$\psi(x) = e^{2\pi i x} \qquad (-.5 \le x \le .5)$$

This has a one-meter wave length and defines a particle whose momentum is known exactly, and whose position is totally uncertain. This is also a stable standing wave on this torus, i.e., a momentum eigenstate. And it is the first momentum eigenstate above the ground state, in which ψ is a constant.

How do we expect this system to behave? According to de Broglie, a particle of mass m with momentum p and energy E undergoing free propagation in one dimension is described by a wave function

$$\psi = \exp[2\pi i(\tau x - \nu t)] = \exp\left[\frac{2\pi i}{h}(px - Et)\right]$$

where

$$\tau = \frac{p}{h} = \text{waves per unit space (wave number)}$$

$$\nu = \frac{E}{h} = \text{waves per unit time (frequency)}$$

It follows that

$$p = \tau h$$

and that

$$E = \frac{p^2}{2m} = \frac{\tau^2 h^2}{2m}$$

Hence

$$\nu = \frac{E}{h} = \frac{h\tau^2}{2m}$$

I.e.,

$$\psi = \exp\left[2\pi i\left(\tau x - \frac{h\tau^2}{2m}t\right)\right] = \exp\left[2\pi i\tau\left(x - \frac{\tau h}{2m}t\right)\right]$$

Thus this wave propagates with speed

$$\frac{\tau h}{2m}$$

which is precisely half of what one would expect from the fact that

$$mv = p = \tau h$$

The program *Schrod* deals with a one dimensional "world" in which the position x goes from $-.5$ to $.5$ with periodic boundary conditions, so that τ must be a positive integer for the value of ψ to wrap continuously around the end of the world. In fact, the initial wave function is the $\tau = 1$ case, and we take $m = 1$ and $\hbar = .1$, so that

$$h = 2\pi\hbar = 6.28\hbar = .628$$

and

$$\psi = \exp[2\pi i(x - (h/2m)t)] = \exp[2\pi i(x - .314t)]$$

Schrod integrates the wave function over t going from 0 to 1. In one unit of time, ψ will propagate a distance of .314 meters. Since we take $\Delta x = 1/50$, this is about sixteen of the fifty cells into which space is divided, which is fortunately what we actually see in the output from *Schrod.*

```
PROBABILITY(POSITION) AT TIME = 0
TOTAL PROBABILITY = 1
-------------------------------------------------------------------------------
| V=0   0 |                                                                  *|
| V=0   1 |                                                                  *|
| V=0   2 |                                                                  *|
| V=0   3 |                                                                  *|
| V=0   4 |                                                                  *|
| V=0   5 |                                                                  *|
| V=0   6 |                                                                  *|
| V=0   7 |                                                                  *|
| V=0   8 |                                                                  *|
| V=0   9 |                                                                  *|
| V=0  10 |                                                                  *|
| V=0  11 |                                                                  *|
| V=0  12 |                                                                  *|
| V=0  13 |                                                                  *|
| V=0  14 |                                                                  *|
| V=0  15 |                                                                  *|
| V=0  16 |                                                                  *|
| V=0  17 |                                                                  *|
| V=0  18 |                                                                  *|
| V=0  19 |                                                                  *|
| V=0  20 |                                                                  *|
| V=0  21 |                                                                  *|
| V=0  22 |                                                                  *|
| V=0  23 |                                                                  *|
| V=0  24 |                                                                  *|
| V=0  25 |                                                                  *|
| V=0  26 |                                                                  *|
| V=0  27 |                                                                  *|
| V=0  28 |                                                                  *|
| V=0  29 |                                                                  *|
| V=0  30 |                                                                  *|
| V=0  31 |                                                                  *|
| V=0  32 |                                                                  *|
| V=0  33 |                                                                  *|
| V=0  34 |                                                                  *|
| V=0  35 |                                                                  *|
| V=0  36 |                                                                  *|
| V=0  37 |                                                                  *|
| V=0  38 |                                                                  *|
| V=0  39 |                                                                  *|
| V=0  40 |                                                                  *|
| V=0  41 |                                                                  *|
| V=0  42 |                                                                  *|
| V=0  43 |                                                                  *|
| V=0  44 |                                                                  *|
| V=0  45 |                                                                  *|
| V=0  46 |                                                                  *|
| V=0  47 |                                                                  *|
| V=0  48 |                                                                  *|
| V=0  49 |                                                                  *|
-------------------------------------------------------------------------------
```

In this and all subsequent graphs of probability as a function of position, zero probability is flush left, and the values have been scaled so that the largest probabilities in any given graph are always flush right.

```
PHASE(POSITION) AT TIME = 0
---------------------------------------------------------
|  V=0   0  |#                                           |
|  V=0   1  | #                                          |
|  V=0   2  |  #                                         |
|  V=0   3  |   #                                        |
|  V=0   4  |   #                                        |
|  V=0   5  |    #                                       |
|  V=0   6  |     #                                      |
|  V=0   7  |      #                                     |
|  V=0   8  |       #                                    |
|  V=0   9  |        #                                   |
|  V=0  10  |         #                                  |
|  V=0  11  |          #                                 |
|  V=0  12  |           #                                |
|  V=0  13  |           #                                |
|  V=0  14  |            #                               |
|  V=0  15  |             #                              |
|  V=0  16  |              #                             |
|  V=0  17  |               #                            |
|  V=0  18  |                #                           |
|  V=0  19  |                 #                          |
|  V=0  20  |                  #                         |
|  V=0  21  |                  #                         |
|  V=0  22  |                   #                        |
|  V=0  23  |                    #                       |
|  V=0  24  |                     #                      |
|  V=0  25  |                      #                     |
|  V=0  26  |                       #                    |
|  V=0  27  |                        #                   |
|  V=0  28  |                         #                  |
|  V=0  29  |                         #                  |
|  V=0  30  |                          #                 |
|  V=0  31  |                           #                |
|  V=0  32  |                            #               |
|  V=0  33  |                             #              |
|  V=0  34  |                              #             |
|  V=0  35  |                               #            |
|  V=0  36  |                                #           |
|  V=0  37  |                                #           |
|  V=0  38  |                                 #          |
|  V=0  39  |                                  #         |
|  V=0  40  |                                   #        |
|  V=0  41  |                                    #       |
|  V=0  42  |                                     #      |
|  V=0  43  |                                      #     |
|  V=0  44  |                                       #    |
|  V=0  45  |                                        #   |
|  V=0  46  |                                        #   |
|  V=0  47  |                                         #  |
|  V=0  48  |                                          # |
|  V=0  49  |                                           #|
---------------------------------------------------------
```

In this and all subsequent graphs of phase as a function of position, phase $-\pi$ is flush left, 0 is in the middle, and $+\pi$ is flush right.

```
PROBABILITY(POSITION) AT TIME    1
TOTAL PROBABILITY     1

|   V=0    0  |                                                       *|
|   V=0    1  |                                                       *|
|   V=0    2  |                                                       *|
|   V=0    3  |                                                       *|
|   V=0    4  |                                                       *|
|   V=0    5  |                                                       *|
|   V=0    6  |                                                       *|
|   V=0    7  |                                                       *|
|   V=0    8  |                                                       *|
|   V=0    9  |                                                       *|
|   V=0   10  |                                                       *|
|   V=0   11  |                                                       *|
|   V=0   12  |                                                       *|
|   V=0   13  |                                                       *|
|   V=0   14  |                                                       *|
|   V=0   15  |                                                       *|
|   V=0   16  |                                                       *|
|   V=0   17  |                                                       *|
|   V=0   18  |                                                       *|
|   V=0   19  |                                                       *|
|   V=0   20  |                                                       *|
|   V=0   21  |                                                       *|
|   V=0   22  |                                                       *|
|   V=0   23  |                                                       *|
|   V=0   24  |                                                       *|
|   V=0   25  |                                                       *|
|   V=0   26  |                                                       *|
|   V=0   27  |                                                       *|
|   V=0   28  |                                                       *|
|   V=0   29  |                                                       *|
|   V=0   30  |                                                       *|
|   V=0   31  |                                                       *|
|   V=0   32  |                                                       *|
|   V=0   33  |                                                       *|
|   V=0   34  |                                                       *|
|   V=0   35  |                                                       *|
|   V=0   36  |                                                       *|
|   V=0   37  |                                                       *|
|   V=0   38  |                                                     *  |
|   V=0   39  |                                                     *  |
|   V=0   40  |                                                     *  |
|   V=0   41  |                                                     *  |
|   V=0   42  |                                                     *  |
|   V=0   43  |                                                     *  |
|   V=0   44  |                                                     *  |
|   V=0   45  |                                                     *  |
|   V=0   46  |                                                     *  |
|   V=0   47  |                                                     *  |
|   V=0   48  |                                                     *  |
|   V=0   49  |                                                     *  |
```

```
PHASE(POSITION) AT TIME = 1
----------------------------------------------------------------
|  V=0   0 |                              #             |
|  V=0   1 |                               #            |
|  V=0   2 |                                #           |
|  V=0   3 |                                 #          |
|  V=0   4 |                                  #         |
|  V=0   5 |                                   #        |
|  V=0   6 |                                   #        |
|  V=0   7 |                                    #       |
|  V=0   8 |                                     #      |
|  V=0   9 |                                      #     |
|  V=0  10 |                                       #    |
|  V=0  11 |                                        #   |
|  V=0  12 |                                         #  |
|  V=0  13 |                                          # |
|  V=0  14 |                                          # |
|  V=0  15 |                                           #|
|  V=0  16 |#                                           |
|  V=0  17 | #                                          |
|  V=0  18 |  #                                         |
|  V=0  19 |   #                                        |
|  V=0  20 |    #                                       |
|  V=0  21 |     #                                      |
|  V=0  22 |      #                                     |
|  V=0  23 |      #                                     |
|  V=0  24 |       #                                    |
|  V=0  25 |        #                                   |
|  V=0  26 |         #                                  |
|  V=0  27 |          #                                 |
|  V=0  28 |           #                                |
|  V=0  29 |            #                               |
|  V=0  30 |             #                              |
|  V=0  31 |             #                              |
|  V=0  32 |              #                             |
|  V=0  33 |               #                            |
|  V=0  34 |                #                           |
|  V=0  35 |                 #                          |
|  V=0  36 |                  #                         |
|  V=0  37 |                   #                        |
|  V=0  38 |                    #                       |
|  V=0  39 |                    #                       |
|  V=0  40 |                     #                      |
|  V=0  41 |                      #                     |
|  V=0  42 |                       #                    |
|  V=0  43 |                        #                   |
|  V=0  44 |                         #                  |
|  V=0  45 |                          #                 |
|  V=0  46 |                           #                |
|  V=0  47 |                           #                |
|  V=0  48 |                            #               |
|  V=0  49 |                             #              |
----------------------------------------------------------------
```

Experiment 2—A Gaussian Wave Packet

There is an intimate and important relationship between the information given in the two parts of each motion picture frame: the graph of the phase indicates the changes which are taking place in the graph of the probability. If the graph of the phase is vertical, that means that ψ is stationary. If the graph of the phase slopes downward to the right, that means that ψ is moving down the page. And if the graph of the phase slopes upward to the right, that means that ψ is moving up the page. In our second experiment, following Goldberg, Schey, and Schwartz, we have a Gaussian wave packet that is simultaneously broadening due to the uncertainty principle, and moving down the page due to its momentum. If it had no momentum and only broadened, the graph of the phase would slope downwards to the right below the peak of the Gaussian, and it would slope upwards to the right above the peak of the Gaussian wave packet, showing that these two halves of the wave packet are moving in opposite directions. Since, however, we have made the wave packet move down the page, the point at which the graph of the phase is vertical lags behind the peak of the Gaussian wave packet, for it occurs at the point at which the backward spreading just balances the forward momentum.

Here is the formula for the initial Gaussian wave packet:

$$\psi(x) \;=\; e^{i\,k_0\,x}\; e^{-\,(x-\,x_0)^2\,/\,2\,\sigma_0^2} \qquad (-.5 \le x \le .5)$$

where

$$\begin{cases} k_0 = 30 \\ x_0 = 0 \\ \sigma_0 = .05 \end{cases}$$

The first exponential gives the wave packet a momentum proportional to k_0, and the second one defines a Gaussian probability distribution with average x_0 and variance σ_0. As this wave packet undergoes free propagation, it retains its shape but broadens, i.e., the variance σ of the Gaussian distribution increases. $k_0' = -\,k_0$ propagates in the opposite direction, and $k_0' = k_0/2$ propagates at half the speed. It can also be shown analytically and verified "experimentally" (that is, via computation) that the rate at which the Gaussian broadens is independent of the speed at which it propagates, i.e., independent of k_0.

The potential energy V is a time independent function of position. In *Schrod* as written, V is identically zero, that is to say, there is no potential and we are looking at a case of free propagation. The program is, however, easily modified to create a square barrier, which illustrates mixed reflection and transmission. It is also easily modified to create an infinite well, which illustrates total reflection. The relevant changes are included in *Schrod* as comments (see line [8]).

Let's now check the extent to which experiment corroborates theory. We shall calculate how fast we expect the Gaussian wave packet to propagate, and then we shall look at the the output from *Schrod* to see how well it agrees with our expectations.

According to de Broglie, the wave number τ and the momentum p are connected as follows

$$\tau = \frac{p}{h}$$

We are working with a world in which the position x goes from $-.5$ to $.5$, and the initial value of the wave function ψ is approximately

$$\psi = \exp[ik_0x] = \exp[2\pi i\tau x]$$

where $k_0 = 30$. It follows that

$$\tau = \frac{k_0}{2\pi} = \frac{30}{2\pi} \approx 5$$

is the number of waves per unit distance, and the wave length is

$$\lambda = \frac{1}{\tau} \approx .2$$

This may be verified by examining the graph of the phase of ψ at time 0 drawn by *Schrod,* which consists as it should of 5 segments. Once we know the wave number τ, the momentum p is determined, for

$$p = h\tau = \frac{hk_0}{2\pi} = \hbar k_0 = .1 \times 30 = 3 \text{ kilogram-meters per second}$$

since $\hbar = .1$ in our toy world. Finally, since $mv = p = 3$ and the mass m is equal to one, it follows that the velocity v is equal to 3 meters per second.

That's the theory. Now let's look at the facts. Examining the output from *Schrod,* we see that at time 0 the peak of the Gaussian wave packet is at point # 25, and it is at point # 37 at time .08. Since our total space of one meter is divided into 50 cells,

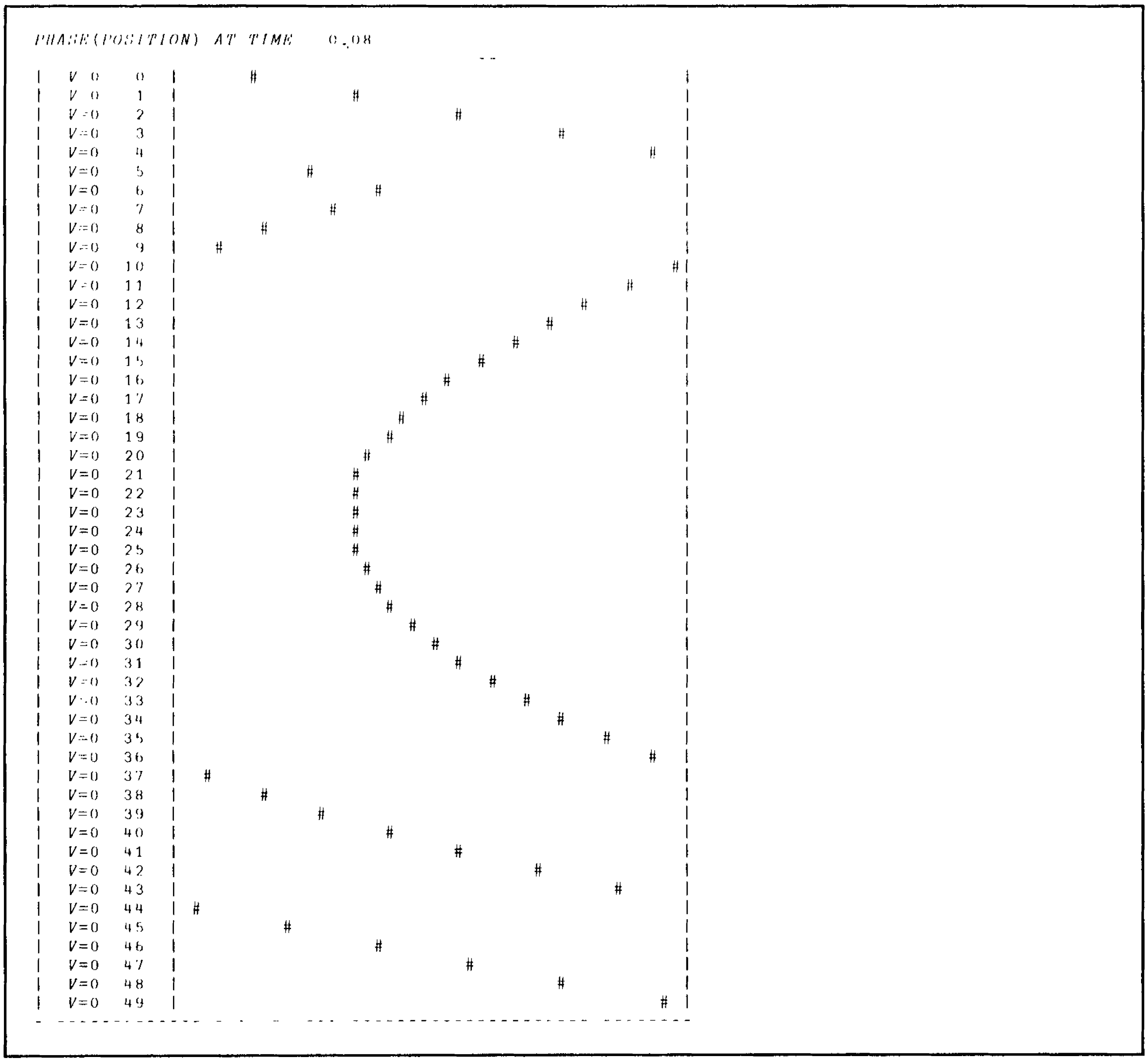
$$\frac{\Delta x}{\Delta t} = \frac{(37 - 25)/50 \text{ space}}{.08 \text{ time}} = \frac{.24 \text{ space}}{.08 \text{ time}} = 3 \text{ meters per second}$$

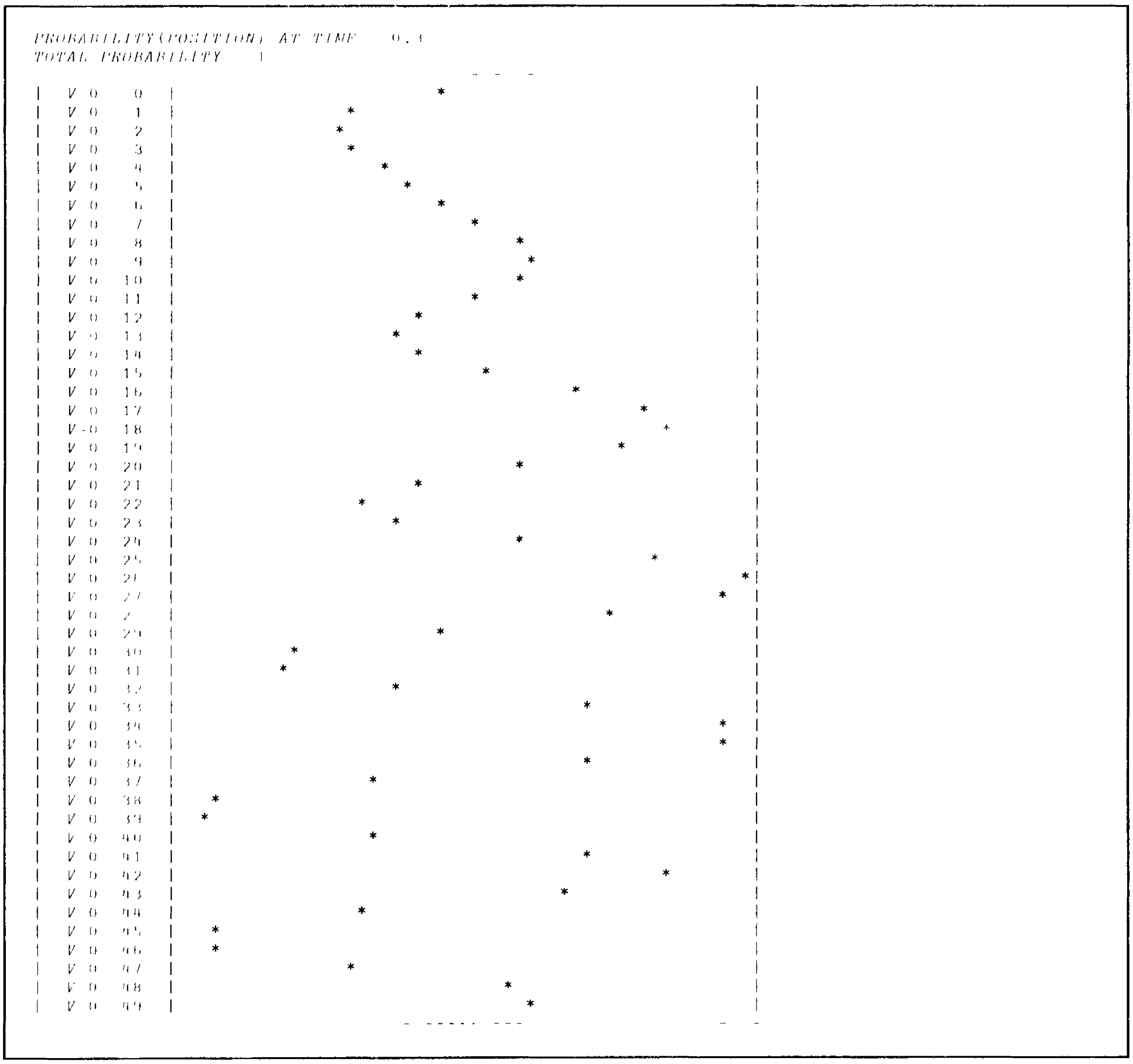
which gives excellent agreement with theory.

```
PROBABILITY(POSITION) AT TIME   0
TOTAL PROBABILITY = 1
|  V=0    0  |*                                                  |
|  V=0    1  |*                                                  |
|  V=0    2  |*                                                  |
|  V=0    3  |*                                                  |
|  V=0    4  |*                                                  |
|  V=0    5  |*                                                  |
|  V=0    6  |*                                                  |
|  V=0    7  |*                                                  |
|  V=0    8  |*                                                  |
|  V=0    9  |*                                                  |
|  V=0   10  |*                                                  |
|  V=0   11  |*                                                  |
|  V=0   12  |*                                                  |
|  V=0   13  |*                                                  |
|  V=0   14  |*                                                  |
|  V=0   15  |*                                                  |
|  V=0   16  |*                                                  |
|  V=0   17  |*                                                  |
|  V=0   18  |*                                                  |
|  V=0   19  |*                                                  |
|  V=0   20  |  *                                                |
|  V=0   21  |       *                                           |
|  V=0   22  |                   *                               |
|  V=0   23  |                                    *              |
|  V=0   24  |                                                  *|
|  V=0   25  |                                                  *|
|  V=0   26  |                                    *              |
|  V=0   27  |                   *                               |
|  V=0   28  |       *                                           |
|  V=0   29  |  *                                                |
|  V=0   30  |*                                                  |
|  V=0   31  |*                                                  |
|  V=0   32  |*                                                  |
|  V=0   33  |*                                                  |
|  V=0   34  |*                                                  |
|  V=0   35  |*                                                  |
|  V=0   36  |*                                                  |
|  V=0   37  |*                                                  |
|  V=0   38  |*                                                  |
|  V=0   39  |*                                                  |
|  V=0   40  |*                                                  |
|  V=0   41  |*                                                  |
|  V=0   42  |*                                                  |
|  V=0   43  |*                                                  |
|  V=0   44  |*                                                  |
|  V=0   45  |*                                                  |
|  V=0   46  |*                                                  |
|  V=0   47  |*                                                  |
|  V=0   48  |*                                                  |
|  V=0   49  |*                                                  |
```

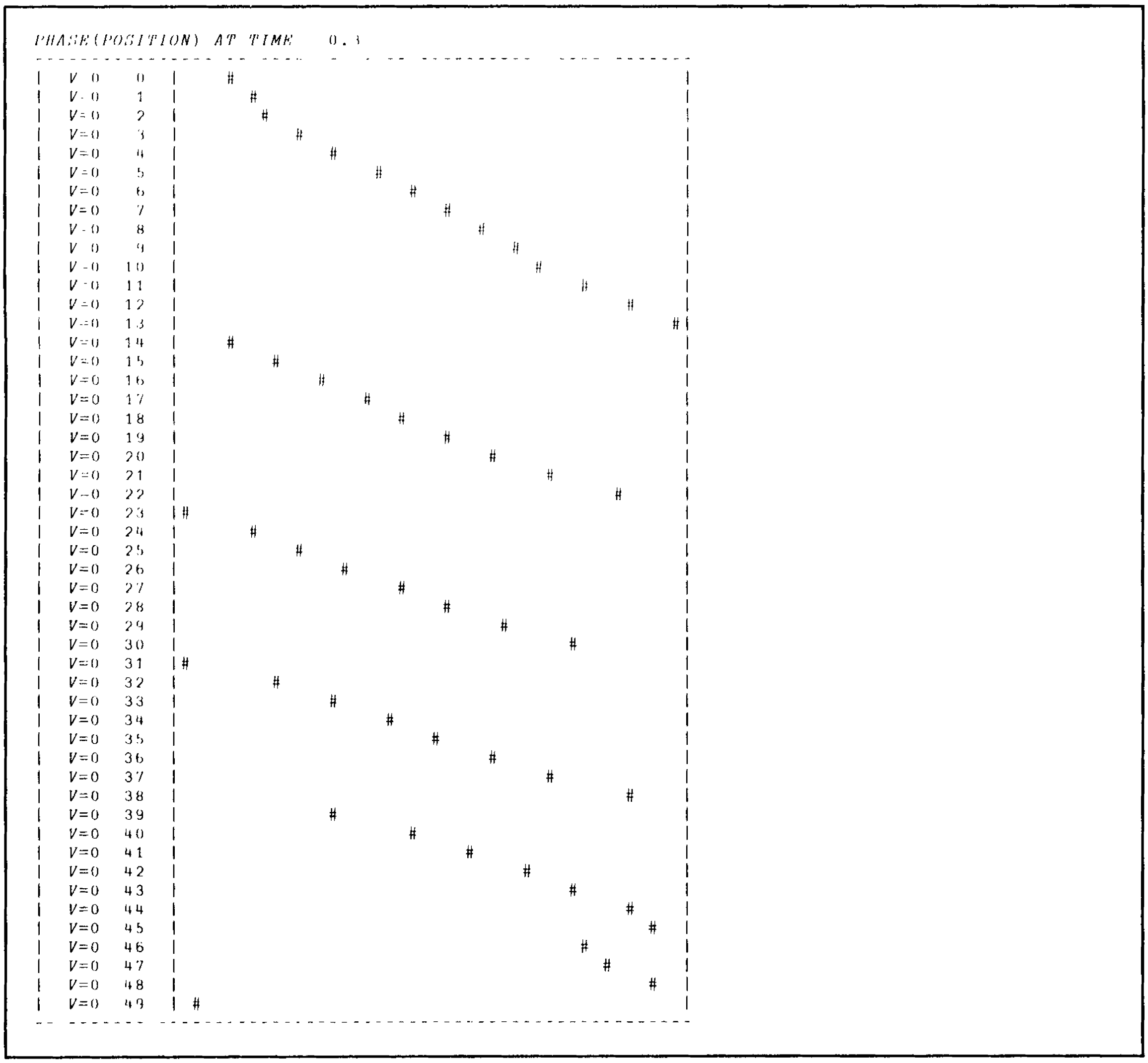
```
PHASE(POSITION) AT TIME   0
-------------------------------------------------------
| V=0  0 |       #                                    |
| V=0  1 |           #                                |
| V=0  2 |               #                            |
| V=0  3 |                   #                        |
| V=0  4 |                       #                    |
| V=0  5 |                            #               |
| V=0  6 |                                #           |
| V=0  7 |                                    #       |
| V=0  8 |                                        #   |
| V=0  9 |#                                           |
| V=0 10 |     #                                      |
| V=0 11 |         #                                  |
| V=0 12 |             #                              |
| V=0 13 |                 #                          |
| V=0 14 |                     #                      |
| V=0 15 |                          #                 |
| V=0 16 |                              #             |
| V=0 17 |                                  #         |
| V=0 18 |                                      #     |
| V=0 19 |                                          # |
| V=0 20 |   #                                        |
| V=0 21 |       #                                    |
| V=0 22 |           #                                |
| V=0 23 |               #                            |
| V=0 24 |                   #                        |
| V=0 25 |                        #                   |
| V=0 26 |                            #               |
| V=0 27 |                                #           |
| V=0 28 |                                    #       |
| V=0 29 |                                        #   |
| V=0 30 | #                                          |
| V=0 31 |     #                                      |
| V=0 32 |         #                                  |
| V=0 33 |             #                              |
| V=0 34 |                 #                          |
| V=0 35 |                      #                     |
| V=0 36 |                          #                 |
| V=0 37 |                              #             |
| V=0 38 |                                  #         |
| V=0 39 |                                      #     |
| V=0 40 |                                           #|
| V=0 41 |   #                                        |
| V=0 42 |       #                                    |
| V=0 43 |           #                                |
| V=0 44 |               #                            |
| V=0 45 |                    #                       |
| V=0 46 |                        #                   |
| V=0 47 |                            #               |
| V=0 48 |                                #           |
| V=0 49 |                                    #       |
-------------------------------------------------------
```

```
PROBABILITY(POSITION) AT TIME    0.08
TOTAL PROBABILITY = 1
-----------------------------------------------------------------
|  V=0    0 |*                                                  |
|  V=0    1 |*                                                  |
|  V=0    2 |*                                                  |
|  V=0    3 |*                                                  |
|  V=0    4 |*                                                  |
|  V=0    5 |*                                                  |
|  V=0    6 |*                                                  |
|  V=0    7 |*                                                  |
|  V=0    8 |*                                                  |
|  V=0    9 |*                                                  |
|  V=0   10 |*                                                  |
|  V=0   11 |*                                                  |
|  V=0   12 |*                                                  |
|  V=0   13 |*                                                  |
|  V=0   14 |*                                                  |
|  V=0   15 |*                                                  |
|  V=0   16 |*                                                  |
|  V=0   17 |*                                                  |
|  V=0   18 |*                                                  |
|  V=0   19 |*                                                  |
|  V=0   20 |*                                                  |
|  V=0   21 | *                                                 |
|  V=0   22 |  *                                                |
|  V=0   23 |   *                                               |
|  V=0   24 |    *                                              |
|  V=0   25 |      *                                            |
|  V=0   26 |        *                                          |
|  V=0   27 |           *                                       |
|  V=0   28 |               *                                   |
|  V=0   29 |                   *                               |
|  V=0   30 |                        *                          |
|  V=0   31 |                             *                     |
|  V=0   32 |                                  *                |
|  V=0   33 |                                       *           |
|  V=0   34 |                                            *      |
|  V=0   35 |                                               *   |
|  V=0   36 |                                                 * |
|  V=0   37 |                                                  *|
|  V=0   38 |                                                *  |
|  V=0   39 |                                           *       |
|  V=0   40 |                                     *             |
|  V=0   41 |                              *                    |
|  V=0   42 |                      *                            |
|  V=0   43 |              *                                    |
|  V=0   44 |        *                                          |
|  V=0   45 |    *                                              |
|  V=0   46 |  *                                                |
|  V=0   47 |*                                                  |
|  V=0   48 |*                                                  |
|  V=0   49 |*                                                  |
```


PHASE(POSITION) AT TIME 0.08



At this time the wave packet has wrapped around the "end of the world," and its forward edge has collided with its trailing edge, producing this interference pattern.


PHASE(POSITION) AT TIME 0.3
V=0 0
V=0 1
V=0 2
V=0 3
V=0 4
V=0 5
V=0 6
V=0 7
V=0 8
V=0 9
V=0 10
V=0 11
V=0 12
V=0 13
V=0 14
V=0 15
V=0 16
V=0 17
V=0 18
V=0 19
V=0 20
V=0 21
V=0 22
V=0 23
V=0 24
V=0 25
V=0 26
V=0 27
V=0 28
V=0 29
V=0 30
V=0 31
V=0 32
V=0 33
V=0 34
V=0 35
V=0 36
V=0 37
V=0 38
V=0 39
V=0 40
V=0 41
V=0 42
V=0 43
V=0 44
V=0 45
V=0 46
V=0 47
V=0 48
V=0 49

Rescaling

We would now like to make these experiments more realistic by rescaling them. In our first experiment we have looked at a "particle" whose mass is one kilogram and whose de Broglie wave length is one meter in a toy world in which $\hbar$ is one-tenth and in which the potential is measured in joules. Let's consider instead the typical quantum mechanical situation of a valence electron. The mass of the electron is 30 orders of magnitude smaller, its wave length is typically measured in angstroms $\mathring{A} = 10^{-10}$ meters, its potential is typically measured in electron volts or eV $= 1.602 \times 10^{-19}$ joules, and $\hbar$ is 33 orders of magnitude smaller. So let's analyze the rescaling necessary if we now consider a typical valence electron and the correct value of $\hbar$.

First we will analyze the rescaling intuitively with physical arguments, and then we will verify this analysis by directly manipulating the Schrödinger equation.

According to de Broglie, the wave length associated with a particle is given by

$$\lambda = \frac{1}{\tau} = \frac{h}{p} = \frac{h}{mv}$$

We took $\lambda' = 1$, $\hbar' = .1$, and $m' = 1$, whereas actual values for a typical valence electron are $\lambda = 10^{-9} = 10\ \mathring{A}$, $\hbar = 1.055 \times 10^{-34} \approx 10^{-34}$ joule-seconds, and $m_e = 9.109 \times 10^{-31} \approx 10^{-30}$ kilograms. I.e., we have multiplied the wave length by a factor of 10^9, the mass by a factor of 10^{30}, and $\hbar$ by a factor of 10^{33}. To compensate for this, let's multiply the velocity by a factor of a 10^6, so that the various correction factors are mutually consistent:

$$(\lambda/\lambda') = \frac{(\hbar/\hbar')}{(m/m')(v/v')} = 10^{-9} = \frac{10^{-33}}{10^{-30} \times 10^{6}}$$

Thus the one meter of space and the one second of time simulated in the computation performed by *Schrod* becomes ten angstroms and $10^{-9} \times 10^{-6} = 10^{-15}$ seconds.

In summary, our calculation applies to the actual electron rest mass and value of Planck's constant in a world 10^{-9} meters long that wraps around, and we have seen that the wave function ψ propagates at $.314 \times 10^6$ meters per second, while the electron which ψ describes has a de Broglie wave length of 10 $\mathring{A}$ and travels at $.628 \times 10^6$ meters per second, i.e., approximately one-five-hundredth the speed of light.

Note that this rescaling also affects the units used to measure the energy and the potential. The kinetic energy of our original one kilogram "particle" was

$$E = \frac{mv^2}{2} \approx \frac{1 \times .628^2}{2} \approx .2 \text{ joules}$$

Since to get a real electron we must multiply the mass m by a factor of 10^{-30} and the velocity v by a factor of 10^6, it follows that the energy E is multiplied by a factor of $10^{-30+6\times 2} = 10^{-18}$. Thus one joule becomes 10^{-18} joules, which is about 6.25 eV. It follows that our calculation corresponds to an electron with an energy of about $.2 \times 6.25 \approx 1.25$ volts.

Now let's rescale our second experiment by the same factors. I.e., we multiply distance by a factor of 10^9, mass by a factor of 10^{30}, $\hbar$ by a factor of 10^{33}, velocity by a factor of a 10^6, time by a factor of 10^{-15}, and energy by a factor of 10^{-18}. Thus the one meter of space and the one second of time simulated in the computation performed by *Schrod* becomes ten angstroms and 10^{-15} seconds, our calculation applies to the actual electron rest mass and value of Planck's constant, and the Gaussian wave packet and its associated electron with a de Broglie wave length of two angstroms, both travel at 3×10^6 meters per second, i.e., approximately one-hundredth the speed of light.

Since it is very interesting to study the propagation of this wave packet in situations in which $V \neq 0$, it is important to note how this rescaling affects the energy and the potential. The kinetic energy of our original one kilogram "particle" was

$$E = \frac{mv^2}{2} \approx \frac{1 \times 3^2}{2} \approx 4.5 \text{ joules}$$

Since the energy E is multiplied by a factor of 10^{-18}, which is about 6.25 eV, it follows that our calculation corresponds to an electron with an energy of about $4.5 \times 6.25 \approx 28$ volts. And if we took the value of the potential V at a point to be one joule, it must actually be 6.25 volts for the result of our calculation to apply to the real m_e and $\hbar$ over ten angstroms of space and 10^{-15} seconds of time.

Now let's rederive these scaling results, by arguing directly from the Schrödinger equation. The equation that we solve numerically is

$$\frac{\partial \psi}{\partial t} = \frac{1}{i \hbar \alpha} \left(- \frac{\hbar^2 \alpha^2}{2 m \beta} \frac{\partial^2 \psi}{\partial (\gamma x)^2} + V \psi \right)$$

where $\alpha \approx 10^{33}$ is the factor by which we multiply the true value of $\hbar$, $\beta \approx 10^{30}$ is the factor by which we multiply the true value of the rest mass of the electron, and $\gamma \approx 10^9$ is the factor by which we multiply the true value of the de Broglie wave length of the electron. I.e., α, β and γ are the scaling factors for $\hbar$, m and x. Hence we have

$$\frac{\partial \psi}{\partial t} = \frac{1}{i \hbar \alpha} \frac{\alpha^2}{\beta \gamma^2} \left(- \frac{\hbar^2}{2 m} \frac{\partial^2 \psi}{\partial x^2} + \left[\frac{\beta \gamma^2}{\alpha^2} \right] V \psi \right)$$

An α cancels out, and we get

$$\frac{\partial \psi}{\partial \left[\frac{\alpha}{\beta \gamma^2} t \right]} = \frac{1}{i \hbar} \left(- \frac{\hbar^2}{2 m} \frac{\partial^2 \psi}{\partial x^2} + \left[\frac{\beta \gamma^2}{\alpha^2} \right] V \psi \right)$$

which is the Schrödinger equation with the correct values of $\hbar$ and m, and with $t' = (\alpha/\beta\gamma^2)\, t$ and $V' = (\beta\gamma^2/\alpha^2)\, V$. Thus the numerical solution of our equation is also a solution of the correct Schrödinger equation over a period of time t' a factor of $\alpha/\beta\gamma^2 \approx 10^{-15}$ times smaller and with potential V' a factor of $\beta\gamma^2/\alpha^2 \approx 10^{-18}$ times smaller.

5. Quantum Field Theory: The Feynman Path Integral and Quantum Electrodynamics as a Lattice Gauge Theory

Gravity is curvature of space-time. And electromagnetism is curvature of the fiber bundle of the phase of the Schrödinger wave function. More precisely, the 4-vector potential corresponds to the connection of general relativity; it tells how to propagate a phase vector from one position to another. This is a beautiful analogy; it is not the unified field theory that Einstein was searching for nor is it a quantum theory of gravity. But it clearly is a high point of contemporary theoretical physics. Unfortunately, I could not devise a program that performs a meaningful quantum electrodynamics calculation, and that would be understandable at the level I am trying to reach. But I believe that the material presented in this booklet can be used to help bring this pinnacle within sight; it helps to make possible a deeper understanding of two excellent recent *Scientific American* articles on gauge theory (Rebbi "Quark Confinement" and Bernstein & Phillips), and it can also be used to help bring within reach some slightly more technical explanations of gauge theory (Moriyasu and Yang).

Readings

- Einstein & Infield, no reading, since this is a subsequent development
- Feynman, Leighton & Sands, on the principle of least action
- Hibbs, on path integrals in quantum mechanics
- Feynman & Hibbs, on path integrals in quantum electrodynamics
- Misner, Thorne & Wheeler, on path integrals in quantum gravity
- Rebbi "Quark Confinement," on lattice gauge theory and Monte Carlo path integrals
- Bernstein & Phillips, on curvature and gauge theory
- Eddington, on Weyl's original gauge theory
- Moriyasu, on gauge theory (more technical)
- Yang, on gauge theory (more technical)
- Mattuck, on many body physics

Additional References

- Creutz & Freedman, for path integrals in imaginary time
- Creutz, Chapter 3, "Path Integrals and Statistical Mechanics," for path integrals in imaginary time
- Maddox, for the Dirac equation as a path integral
- Gaveau, Jacobson, Kac & Schulman, for the Dirac equation as a path integral
- Jacobson & Schulman, for the Dirac equation as a path integral
- Rebbi, *Lattice Gauge Theories*
- Schulman

Feynman—Nonrelativistic Quantum Mechanics in One Dimension

```
      )LOAD FEYNMAN
SAVED 1985-01-16 18.44.24 (GMT-5) 2727K(2663K)

      ∇FEYNMAN[⎕]∇
[ 0]   FEYNMAN
[ 1]   ⎕IO←0
[ 2]   I←0J1
[ 3]   HBAR←.1
[ 4]   MASS←1
[ 5]   DELX←DELT←1÷N←20
[ 6]   X←¯.5+(.5+⍳N)÷N
[ 7]   V←Nρ0
[ 8]   K0←(⍳N)∘.PROP⍳N
[ 9]   K←⊃+.×/Nρ⊂K0
[10]   0 DRAW PSI←*(○2)×I×X
[11]   1 DRAW K+.×PSI

      ∇PROP[⎕]∇
[0]   PROP←M PROP M0 ⍝ AMPLITUDE TO PROPAGATE TO CELL M FROM CELL M0
[1]   SPEED←(DELX×(|M-M0)⌊(N-|M-M0))÷DELT
[2]   KE←.5×MASS×SPEED*2
[3]   PE←.5×V[M]+V[M0]              ⍝ TO GO TO IMAGINARY TIME,
[4]   PROP←*I×(KE-PE)×DELT÷HBAR ⍝ PROP←*-(KE+PE)×DELT÷HBAR

      ∇DRAW[⎕]∇
[0]   TIME DRAW PSI
[1]   ' '
[2]   'PROBABILITY(POSITION) AT TIME = ',⍕TIME
[3]   'TOTAL PROBABILITY = ',⍕+/PROB←|PSI*2
[4]   FRAME(-⌊50×PROB÷⌈/PROB)⌽(N 51ρ'*',50ρ' ')
[5]   ' '
[6]   'PHASE(POSITION) AT TIME = ',⍕TIME
[7]   FRAME(-⌊22+7×11○⍟(PSI=0)+PSI)⌽(N 44ρ'#',43ρ' ')

      ∇FRAME[⎕]∇
[0]   FRAME PIC
[1]   PIC←(N 5ρ'|  V='),(⍕N 1ρV),' ',' ',(⍕N 1ρ⍳N),' ',' ','|',PIC,'|'
[2]   '-',[0]PIC,[0]'-'
```

This program treats a one-dimensional non-relativistic quantum mechanical situation via a Feynman integral over all paths = a sum over all histories. We use Feynman's original formulation, in which time is real.

According to Feynman, the amplitude to get from position a at time t_a to position b at time t_b is given by the following integral over all paths $x(t)$ such that $x(t_a) = a$ and $x(t_b) = b$:

$$K(b,\ t_b,\ a,\ t_a) \ = \ \int_{x(t_a)=a}^{x(t_b)=b} e^{i\, S(b,\, a)/\hbar} \ dx(t)$$

Here $\hbar$ is Planck's constant divided by 2π (its numerical value is actually 1.055×10^{-34} joule-sec), and $S(b, a)$ is the action over the path from a to b. The action is defined as follows:

$$S(b,\ a) \ = \ \int_{t_a}^{t_b} (KE - PE)\, dt$$

Here KE = kinetic energy and PE = potential energy. Thus the action S is also $(t_b - t_a)$ times (the expected value of $KE - PE$).

Note that the Feynman approach in a sense includes that of Schrödinger. Let us define $\psi(x, t)$ to be the amplitude to be at position x at time t, starting from anywhere at time $-\infty$. Then we can use the so-called "propagator" K to express in integral form Schrödinger's equation for the time evolution of the wave function ψ:

$$\psi(x, t') \ = \ \int_{-\infty}^{+\infty} K(x, t', y, t)\ \ \psi(y, t)\ \ dy$$

The usual differential form of the Schrödinger equation is obtained as the limit of

$$\psi(x, t + \varepsilon) \ = \ \int_{-\infty}^{+\infty} K(x, t + \varepsilon, y, t)\ \ \psi(y, t)\ \ dy$$

as ε tends to zero.

In order to obtain a finite number of paths, we limit ourselves to positions between $-.5$ and $.5$ and to times between 0 and 1, and we divide the space from $-.5$ to $.5$ into N cells, and the time from 0 to 1 into N intervals, so that $\Delta x = \Delta t = 1/N$. At this level of granularity, there are N^N possible paths. Thus our goal is to calculate the $N \times N$ propagator matrix $K(x', x)$ = the amplitude to reach cell x' from cell x in unit time, by summing over all N^N possible paths in the manner prescribed by Feynman. In order to do this, we shall start by calculating $K_0(x', x)$ = the amplitude to reach cell x' from cell x in time Δt.

It fortunately turns out that we can integrate over all N^N paths, with only N^4 amount of work. This is done by raising the infinitesimal propagator matrix K_0 to the Nth matrix power to get the matrix K. This procedure is justified by the equation

$$K(z,\ t + 2\Delta t,\ x,\ t) \ = \ \int_{-\infty}^{+\infty} K(z,\ t + 2\Delta t,\ y,\ t + \Delta t)\ \ K(y,\ t + \Delta t,\ x,\ t)\ \ dy$$

which states that the amplitude to get from x to z in time $2\Delta t$ is the sum of the product of the amplitudes taken over all intermediate points in the path y; this is essentially the rule for matrix multiplication.

But how can we calculate K_0? In order to do this, we must be able to estimate the Lagrangian $L = KE - PE$ in a segment of a path in which the particle has moved from position x to x' in time Δt. The obvious estimate is:

$$L \ \approx \ \frac{mv^2}{2} - V \ \approx \ \frac{m\,|x' - x|^2}{2\,(\Delta t)^2} - \frac{V(x') + V(x)}{2}$$

But taking into account the periodic boundary conditions, we see that in this estimate $|x' - x|$ should be replaced by

$$\min \quad |x' - x|, \quad 1 - |x' - x|$$

since it may be shorter to get from x to x' by going in the opposite direction and wrapping around our toy world which is only one unit in length.

Now for test data. First we must decide on the potential energy V as a function of position, which we have assumed to be time independent. We shall consider the case of free propagation, i.e., no forces are acting on the particle, and take V to be identically zero:

$$V = 0$$

Next we must pick an initial wave function ψ to which to apply the propagator K in order to determine how ψ looks after unit time. We choose a very simple case, an eigenfunction or standing wave in which the particle has precise momentum and totally uncertain position:

$$\psi(x) = e^{2\pi i x} \quad (-.5 \leq x \leq .5)$$

```
PROBABILITY(POSITION) AT TIME    0
TOTAL PROBABILITY    20
                                                                    -----
|  V=0    0  |                                                           *|
|  V=0    1  |                                                           *|
|  V=0    2  |                                                           *|
|  V=0    3  |                                                           *|
|  V=0    4  |                                                           *|
|  V=0    5  |                                                           *|
|  V=0    6  |                                                           *|
|  V=0    7  |                                                           *|
|  V=0    8  |                                                           *|
|  V=0    9  |                                                           *|
|  V=0   10  |                                                           *|
|  V=0   11  |                                                           *|
|  V=0   12  |                                                           *|
|  V=0   13  |                                                           *|
|  V=0   14  |                                                           *|
|  V=0   15  |                                                           *|
|  V=0   16  |                                                           *|
|  V=0   17  |                                                           *|
|  V=0   18  |                                                           *|
|  V=0   19  |                                                           *|

PHASE(POSITION) AT TIME    0

|  V=0    0  | #                                             |
|  V=0    1  |   #                                           |
|  V=0    2  |     #                                         |
|  V=0    3  |       #                                       |
|  V=0    4  |         #                                     |
|  V=0    5  |            #                                  |
|  V=0    6  |              #                                |
|  V=0    7  |                #                              |
|  V=0    8  |                  #                            |
|  V=0    9  |                    #                          |
|  V=0   10  |                       #                       |
|  V=0   11  |                         #                     |
|  V=0   12  |                           #                   |
|  V=0   13  |                             #                 |
|  V=0   14  |                               #               |
|  V=0   15  |                                  #            |
|  V=0   16  |                                    #          |
|  V=0   17  |                                      #        |
|  V=0   18  |                                        #      |
|  V=0   19  |                                          #    |
```

```
PROBABILITY(POSITION) AT TIME - 1
TOTAL PROBABILITY = 2.148530194E17
-------------------------------------------------------------------
|  V=0   0 |                                                  *  |
|  V=0   1 |                                                  *  |
|  V=0   2 |                                                  *  |
|  V=0   3 |                                                  *  |
|  V=0   4 |                                                  *  |
|  V=0   5 |                                                   * |
|  V=0   6 |                                                  *  |
|  V=0   7 |                                                  *  |
|  V=0   8 |                                                  *  |
|  V=0   9 |                                                  *  |
|  V=0  10 |                                                  *  |
|  V=0  11 |                                                  *  |
|  V=0  12 |                                                  *  |
|  V=0  13 |                                                  *  |
|  V=0  14 |                                                  *  |
|  V=0  15 |                                                  *  |
|  V=0  16 |                                                  *  |
|  V=0  17 |                                                  *  |
|  V=0  18 |                                                  *  |
|  V=0  19 |                                                  *  |
-------------------------------------------------------------------

PHASE(POSITION) AT TIME   1
-----------------------------------------------------------
|  V=0   0 |                      #                       |
|  V=0   1 |                        #                     |
|  V=0   2 |                          #                   |
|  V=0   3 |                            #                 |
|  V=0   4 |                               #              |
|  V=0   5 |                                 #            |
|  V=0   6 |                                   #          |
|  V=0   7 |                                     #        |
|  V=0   8 |                                       #      |
|  V=0   9 |                                          #   |
|  V=0  10 |                                            # |
|  V=0  11 | #                                            |
|  V=0  12 |   #                                          |
|  V=0  13 |     #                                        |
|  V=0  14 |        #                                     |
|  V=0  15 |          #                                   |
|  V=0  16 |            #                                 |
|  V=0  17 |              #                               |
|  V=0  18 |                #                             |
|  V=0  19 |                   #                          |
-----------------------------------------------------------
```

Note that the total probability is outrageously different from one. We have already calculated what the value of ψ should be after unit time by using the Schrödinger equation (experiment 1 in the previous chapter); our result this time differs from the previous one by a large complex normalization factor. Going to imaginary time improves convergence and makes normalization trivial, but the physical interpretation of the mathematics is then much more subtle.

Postscript

Before posing some queries, we cannot help expressing our amazement that a significant portion of the spirit of fundamental physics has in some sense been captured in six pages of APL. In particular, our calculation of the Ricci tensor is hardly more than half a page. Partly this is a tribute to APL—but there are deeper issues involved. Speaking as a computer programmer who has worked with large COBOL, RPG, and assembly language commercial programs, and speaking as a systems programmer who has been involved with optimizing compilers and operating systems, I am struck by the fact that general relativity is in some sense captured by a program of such small size. This program is minute compared to any real useful computer program that I have ever dealt with. The moral is, I believe, that general relativity is simple compared, for example, to the complexity of human society as mirrored in the size of the computer programs which service it. Indeed, the beauty of some of the fundamental ideas of theoretical physics is precisely that they are so simple and yet at the same time so powerful and far-reaching.

This enterprise also raises questions of a more fundamental nature. There is a school of foundational thought in mathematics that maintains that what cannot be computed does not exist; this constructivist foundational tendency in mathematics suggests that there is perhaps more to the computer based approach to physics than meets the eye. Do real numbers with their infinity of decimal digits really exist, or is space-time ultimately discrete and finite? Is it possible that the universe is really a giant computer or a cellular automaton, as Edward Fredkin believes? Turning to the more mundane, can computational complexity theory be applied to physics and used to give lower bounds on the computational effort required to do physics, and maybe even to show that some physical computations are inherently inaccessible no matter what method is used to calculate them? Path integrals for fields are terribly time consuming, even if Monte Carlo approximation (sampling) is used. It would be terribly frustrating if physics were to expose the innermost mechanism of the world and this proved to be quite simple, but it turned out to be impossible to ever calculate from it how anything of interest worked!

I would like to end by telling a joke that R. D. Mattuck attributes to G. E. Brown about the manner in which physics progresses. In Newtonian physics the two-body problem has an exact analytical solution, the ellipse, but the three-body problem (earth-moon-sun) can only be approximated numerically. In general relativity the one-body problem can be solved exactly (the Schwarzschild metric), but the two-body problem seems too difficult. Finally in quantum field theory, the zero-body problem or vacuum is already too hard to solve! In fact the vacuum is such a hotbed of activity that according to some reckonings its energy is infinite—can this be right, ask Feynman & Hibbs?

Readings

- Chaitin, on the size of programs as a measure of complexity
- Feynman, on how can an infinite amount happen in an infinitesimal cube
- Wolfram, on physical calculations lacking computational shortcuts
- Mattuck, on how many bodies it takes to have a problem
- Feynman & Hibbs, on the energy of the quantum electrodynamic vacuum
- Series of three special issues on the physics of computation in the *International Journal of Theoretical Physics*, vol. 22 (1982)

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