

The Journal of Undergraduate Research in Physics

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FINITE ELEMENT SOLUTION OF THE SCHRODINGER EQUATION FOR THE HYDROGEN ATOM

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ABSTRACT

The Finite Element Method is a numerical technique for solving second order differential equations with boundary conditions. The method was developed in the 1950's for solving problems in stress analysis. However, it has great potential for use in physics where most equations must be solved by approximation. In this paper, the Finite Element Method is applied to the radial equation of the hydrogen atom to provide an analytic standard with which to compare the numerical results. This paper is divided into three parts. Part 1 describes the analytic solution of the radial equation, part 2 the finite element solution and part 3 is a comparison of analytic and numerical results as well as a discussion of errors.

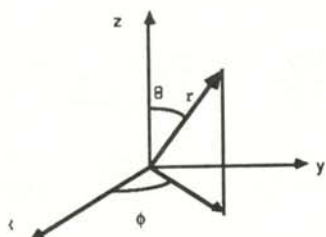
ANALYTIC SOLUTION OF THE RADIAL EQUATION

The time independent Schrodinger equation for the hydrogen atom in atomic units is:

$$\nabla^2 \Psi + 2 \left(E + \frac{1}{r} \right) \Psi = 0, \quad (1)$$

subject to the boundary conditions that

$$\Psi(r \rightarrow \infty) \rightarrow 0.$$



In atomic units, $h/2\pi = m = e = 1$, the unit of distance is the Bohr radius $a_0 = h^2/4\pi^2 m e^2$

FIGURE 1
Spherical Coordinates

and the unit of energy is in a.u. $= 4\pi^2 m e^4 / h^2$.

For spherically symmetric potentials, $V = V(r)$, it is advantageous to use spherical coordinates (see Figure 1) where the Laplacian is expressed as:

$$\nabla^2 = \frac{1}{r^2} \frac{d}{dr} \left[r^2 \frac{d}{dr} \right] + \frac{1}{r^2 \sin^2 \theta} \frac{d^2}{d\phi^2} + \frac{1}{r^2 \sin \theta} \frac{d}{d\theta} \left[\sin \theta \frac{d}{d\theta} \right] \quad (2)$$

or

$$\nabla^2 = \frac{1}{r^2} \frac{d}{dr} \left[r^2 \frac{d}{dr} \right] - \frac{L^2}{r^2}, \quad (3)$$

where L^2 is the angular momentum operator.

The wave function can then be expressed as a product of a function of the radius r and a function of the angles.

$$\Psi(r, \theta, \phi) = R(r) Y(\theta, \phi) \quad (4)$$

Substituting Equation 2 and Equation 4 into Equation 1 and multiplying through by r^2/YR , one obtains:

$$\frac{1}{R} \left\{ \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \frac{1}{Y \sin \theta} \frac{d}{d\theta} \left[\sin \theta \frac{dY}{d\theta} \right] + \frac{1}{\sin^2 \theta} \frac{d^2 Y}{d\phi^2} \right\} + 2 \left[E + \frac{1}{r} \right] r^2 = 0. \quad (5)$$

Separating radial functions on the left and the angular functions on the right yields:

$$\frac{1}{R} \left\{ \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + 2 \left[E + \frac{1}{r} \right] r^2 R \right\} = -\frac{1}{Y} \left\{ \frac{1}{\sin \theta} \frac{d}{d\theta} \left[\sin \theta \frac{dY}{d\theta} \right] + \frac{1}{\sin^2 \theta} \frac{d^2 Y}{d\phi^2} \right\}. \quad (6)$$

The left and right are independent of each other and hence, are equal to some constant. The angular equation is further separated and the solution to the differential equation in θ and ϕ is the spherical harmonics, $Y_l^m(\theta, \phi)$, where l is an integer ≥ 0 and $-l < m < l$. This determines the constant for Equation 6 and one obtains the radial equation:

$$-\frac{1}{2r^2} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \left\{ \frac{l(l+1)}{2r^2} - \frac{1}{r} \right\} R = ER \quad (7)$$

This equation can be solved exactly for the eigenvalue E_n and the corresponding normalized eigenstates $R_{n,l}$

$$R_{nl}(r) = -2 \left[\frac{1}{n} \right]^{\frac{3}{2}} \sqrt{\frac{(n-l-1)!}{n(n+l)!}} \left[\frac{2r}{n} \right]^l \exp\left(-\frac{r}{n}\right) L_{n+l}^{2+l}\left(\frac{2r}{n}\right) \quad (8)$$

where $E_n = -1/2n^2$ and the L 's are the Laguerre polynomials. ¹ The eigen pairs for several values of n are given in Table 1.

n	l	E (au.)	$R_{n,l}$
1	0	-0.5	$2e^{-r}$
2	0	-0.125	$\left[\frac{1}{2}\right]^{\frac{3}{2}} (2-r) \exp\left(-\frac{r}{2}\right)$
	1		$\left[\frac{1}{2}\right]^{\frac{3}{2}} \frac{1}{\sqrt{3}} r \exp\left(-\frac{r}{2}\right)$
3	0	-0.05	$\left[\frac{1}{3}\right]^{\frac{3}{2}} 2 \left\{ 1 - \frac{2}{9} r + \frac{2}{27} r^2 \right\} \exp(-r/3)$
	1		$\left[\frac{1}{3}\right]^{\frac{3}{2}} \frac{4\sqrt{2}}{9} r \left\{ 1 - \frac{r}{6} \right\} \exp(-r/3)$
	2		$\left[\frac{1}{3}\right]^{\frac{3}{2}} \frac{2}{27} \sqrt{\frac{2}{15}} r^2 \exp(-r/3)$

TABLE 1

Analytic form of the radial solutions to the hydrogen atom for $n = 1, 2$ and 3

FINITE ELEMENT APPROACH

The finite element method ² will now be applied to find a numerical solution to the radial part of Schrodinger's equation for the hydrogen atom. Equation 7 is then rewritten as:

$$-\frac{d^2 R}{dr^2} - \frac{2}{r} \frac{dR}{dr} + \frac{l(l+1)}{r^2} R - \frac{2}{r} R = 2ER \quad (9)$$

In finite element analysis, one multiplies through by $r^2 R(r)$ and integrates over r :

$$\int \left[-R \frac{d^2 R}{dr^2} - R \frac{2}{r} \frac{dR}{dr} + R \frac{l(l+1)}{r^2} - R \frac{2}{r} R \right] r^2 dr = 2E \int R R r^2 dr \quad (10)$$

The integration is weighted by r^2 since this corresponds to a volume integral in spherical coordinates. Integrating by parts, one obtains:

$$\int \left[\frac{dR}{dr} \frac{dR}{dr} - R \frac{2}{r} R + R \frac{l(l+1)}{r^2} R \right] r^2 dr = 2E \int R R r^2 dr \quad (11)$$

Since the range of integrations is 0 to ∞ , one must choose some suitable cutoff value r_c , where $R(r = r_c) = 0$.

The coordinate space r is now divided into N discrete subdivisions called finite elements. The two points which form the boundary of the element and the midpoint of each element are called nodes or nodal points. In each element nel of length h^{nel} , a local coordinate system is introduced. The local coordinate x , which ranges from 0 to 1, is related to the global coordinate r by:

$$r = r_0^{nel} + h^{nel} x, \quad (12)$$

where r_0^{nel} is the global value of r at the left node in the local element nel . Using

$$\frac{d}{dr} = \frac{1}{h^{nel}} \frac{d}{dx}, \quad (13)$$

and

$$\int_0^{r_c} dr = \sum_{nel=1}^N h^{nel} \int_0^1 dx, \quad (14)$$

the local coordinate representation of the radial equation for element nel is:

$$h^{nel} \int_0^1 \left[\frac{1}{(h^{nel})^2} \frac{dR^{nel}}{dx} \frac{dR^{nel}}{dx} - \frac{2 R^{nel} R^{nel}}{(r_0^{nel} + h^{nel} x)} + R^{nel} R^{nel} \frac{l(l+1)}{(r_0^{nel} + h^{nel} x)^2} \right] (r_0^{nel} + h^{nel} x)^2 dx = 2 h^{nel} \int_0^1 E R^{nel} R^{nel} (r_0^{nel} + h^{nel} x)^2 dx \quad (15)$$

From this point on, the superscript 'nel' on h , R and r_0 will be suppressed. It should be understood, however, that these constants are element-dependent.

In each element, the radial wave function R is expanded in terms of the Lagrange polynomials $\phi_i(x)$:

$$R(x) = \sum_{i=1}^3 R_i \phi_i(x) \quad (16)$$

$\phi_i(x)$ is chosen such that R_i is the numerical value of the function R at the node i of the element nel .

The Lagrange polynomial basis functions are:

$$\begin{aligned} \phi_1 &= 1 - 3x + 2x^2 \\ \phi_2 &= 4(x - x^2) \\ \phi_3 &= -x + 2x^2 \end{aligned} \quad (17)$$

Note that:

$$\begin{aligned} \phi_1(0) &= \phi_2(.5) = \phi_3(1) = 1 \\ \phi_1(.5) &= \phi_1(1) = \phi_2(0) = 0 \\ \phi_2(1) &= \phi_3(0) = \phi_3(.5) = 0 \end{aligned} \quad (18)$$

Substituting Equation 16 into Equation 15 for a single element, one obtains:

$$h \int_0^1 \sum_{i=1}^3 \sum_{j=1}^3 \left[\frac{1}{h^2} R_i \phi_i' R_j \phi_j' - \frac{2}{(r_0 + hx)} R_i \phi_i R_j \phi_j + \frac{l(l+1)}{(r_0 + hx)} R_i \phi_i R_j \phi_j \right] (r_0 + hx)^2 dx = 2h \int_0^1 \sum_{i=1}^3 \sum_{j=1}^3 E R_i \phi_i R_j \phi_j (r_0 + hx)^2 dx \quad (19)$$

The terms $(r_0 + hx)$ and $(r_0 + hx)^2$ are now expanded in terms of the Lagrange Polynomials:

$$(r_0 + hx) = \sum_{k=1}^3 \alpha_k \phi_k \quad (20)$$

$$(r_0 + hx)^2 = \sum_{k=1}^3 \beta_k \phi_k \quad (21)$$

where these expansion coefficients are known.

Equation 19 can now be written as:

$$h \sum_{i=1}^3 \sum_{j=1}^3 \int_0^1 \left[\frac{1}{h^2} R_i \phi_i' R_j \phi_j' \left(\sum_{k=1}^3 \beta_k \phi_k \right) - 2 R_i \phi_i R_j \phi_j \left(\sum_{k=1}^3 \alpha_k \phi_k \right) + l(l+1) R_i \phi_i R_j \phi_j \right] dx \quad (22)$$

$$= 2h E \sum_{i=1}^3 \sum_{j=1}^3 \int_0^1 R_i \phi_i R_j \phi_j \left(\sum_{k=1}^3 \beta_k \phi_k \right) dx$$

Note that all the integration now involves simple polynomials which can be done exactly. R_i and R_j are the unknown expansion coefficients for the wave function, and are independent of the variable

x , so they may be removed from the integration:

$$h \sum_{i=1}^3 \sum_{j=1}^3 R_i \int_0^1 \left[\frac{1}{h^2} \phi_i' \phi_j' \left(\sum_{k=1}^3 \beta_k \phi_k \right) - 2 \phi_i \phi_j \left(\sum_{k=1}^3 \alpha_k \phi_k \right) + l(l+1) \phi_i \phi_j \right] dx R_j = \quad (23)$$

$$2h E \sum_{i=1}^3 \sum_{j=1}^3 R_i \left[\int_0^1 \phi_i \phi_j \left(\sum_{k=1}^3 \beta_k \phi_k \right) dx \right] R_j$$

If one defines the following local matrices for the element nel :

$$H_{ij} = h \int_0^1 \left[\frac{1}{h^2} \phi_i' \phi_j' \left(\sum_{k=1}^3 \beta_k \phi_k \right) - 2 \phi_i \phi_j \left(\sum_{k=1}^3 \alpha_k \phi_k \right) + l(l+1) \phi_i \phi_j \right] dx \quad (24)$$

$$U_{ij} = h \int_0^1 \phi_i \phi_j \left(\sum_{k=1}^3 \beta_k \phi_k \right) dx \quad (25)$$

Equation 23 then can be represented in matrix notation as:

$$R_i H_{ij} R_j = R_i E U_{ij} R_j \quad (26)$$

where the unknown constant E and the eigen vectors R can be found by solving the 3×3 eigen value problem:

$$\begin{bmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{bmatrix} \begin{bmatrix} R_1 \\ R_2 \\ R_3 \end{bmatrix} = E \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{bmatrix} \begin{bmatrix} R_1 \\ R_2 \\ R_3 \end{bmatrix} \quad (27)$$

r_c a_0	N	E_1	E_2 (a.u.)	E_3
6	6	-0.4987	+0.0121	+0.6351
6	12	-0.4992	+0.0127	+0.6319
6	18	-0.4993	+0.0127	+0.6319
12	6	-0.4948	-0.1206	+0.0212
12	12	-0.4995	-0.1213	+0.0987
12	18	-0.4995	-0.1214	+0.0198
18	6	-0.4816	-0.1225	+0.0431
18	12	-0.4995	-0.1249	-0.0446
18	18	-0.4995	-0.1249	-0.0460
21	42	-0.5000	-0.1250	-0.0515
EXACT		-0.5000	-0.1250	-0.0555

TABLE 2

Results for the energy eigen value for principle quantum numbers 1,2 and 3 using finite element techniques.

The eigen vectors corresponding to the wave function were also calculated. For six elements, the finite element approximation of the wavefunction for $n = 1$ closely approximated the real curve (see Figure 4). Because the matrix calculations involved the use of double precision variables and the size of the global matrices grew with increasing numbers of elements, the computer time needed to do calculations for high n and large numbers of elements rose drastically.

The calculations for the excited states, where the wave function was more extended in space and had more structure, more nodes were required and the cutoff value of r was increased. The results (see figure 5) for $n = 1, 2$ and 3 and the corresponding allowed values of angular momentum were calculated with 42 elements. The agreement of the approximation and the analytic solutions is noteworthy.

ACKNOWLEDGMENTS

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2. Zienkiewicz, O.C., The Finite Element Method, 3rd Edition, McGraw-Hill Book Company (UK) Ltd., New York, 1977.
3. Bathe, K., and E.L. Wilson, Numerical Methods in Finite Element Analysis, Prentice-Hall, Englewood Cliffs, NJ, 1982, pp. 1 - 63.
4. A listing of the FORTRAN program may be obtained by writing to: Mathieu Massicotte, Box 13, Portsmouth Abbey School, Portsmouth, RI, 02871.

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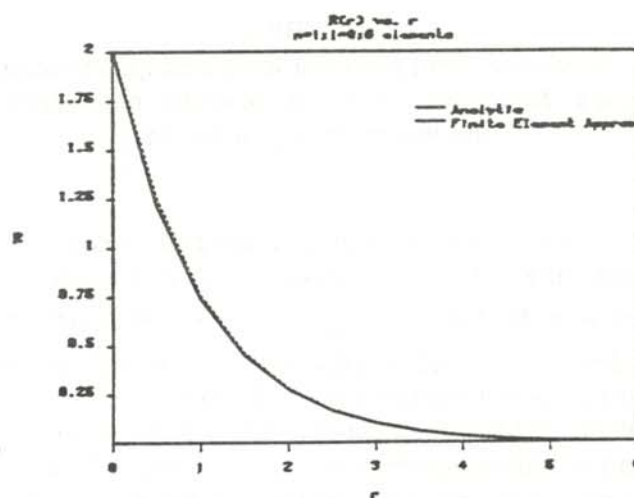


FIGURE 4

Comparison of the finite element approximation with 6 elements and the analytic solution for $n = 1$

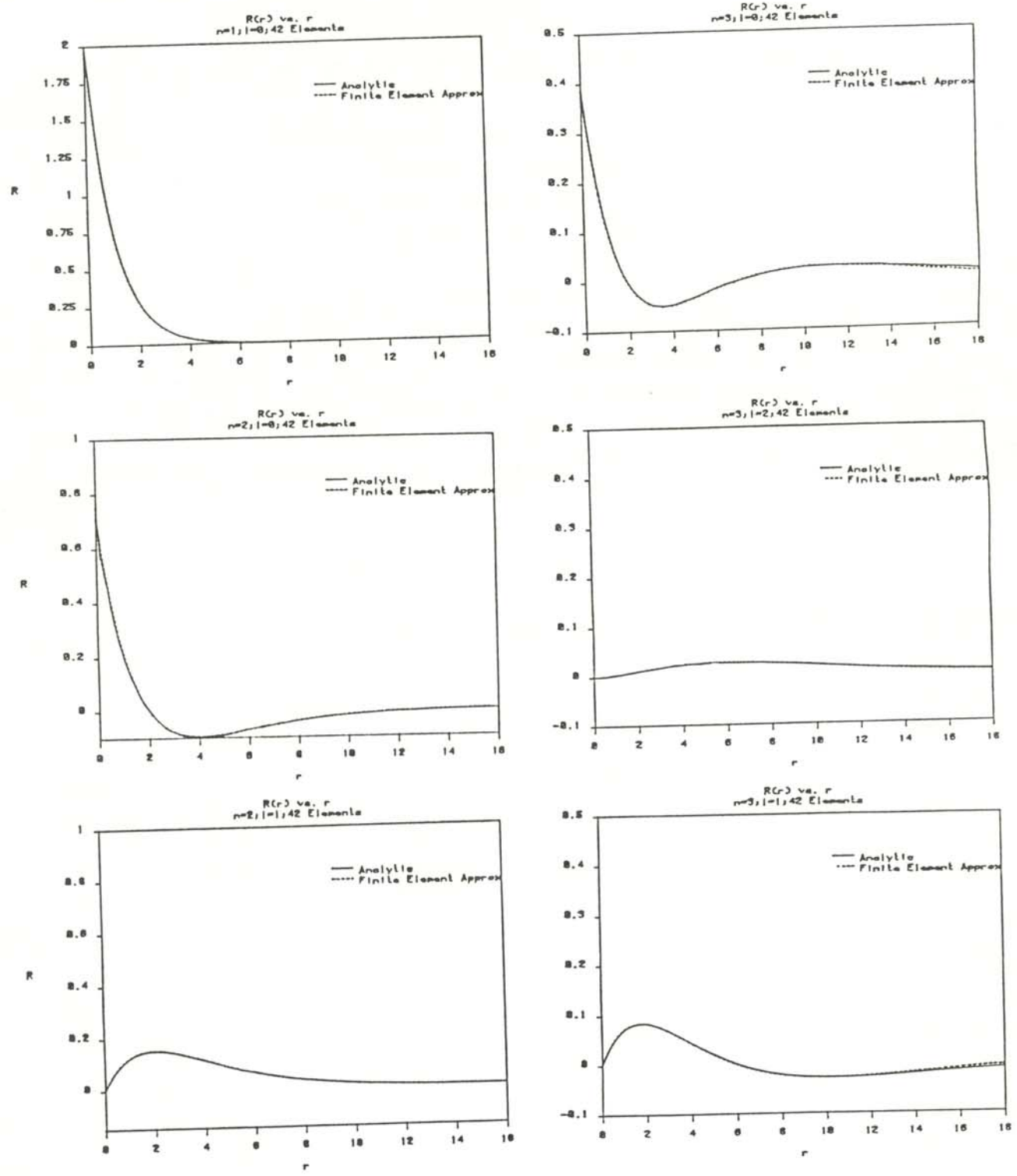


FIGURE 5

The graphed results of the finite element numerical analysis of the radial solutions of the hydrogen atom compared to the analytical solutions. The calculations were done with 42 elements.

THE SPEED OF SOUND - STILL AIR VS. MOVING AIR

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ABSTRACT

This experiment determined how the speed of sound changed in moving air. An interface with the Commodore 64 Computer was constructed and used to measure the change in the speed of sound. A paper tube was used to provide the environment needed to control the flow and velocity of the air. The speed of sound was observed to increase proportionally with increased air flow. The data was fit by the equation:

$$\text{Speed of Sound} = \text{SASS} + 0.3 W$$

where SASS is the Still Air Sound Speed and W is the wind speed measured in meters per second.

BACKGROUND

Sound travels in longitudinal pressure waves (see Figure 1) in any medium, regardless of the material. The sound travels through the medium in a wave that increases and decreases the density of the medium. If the medium moves in the same direction as the sound, the speed of sound will in-

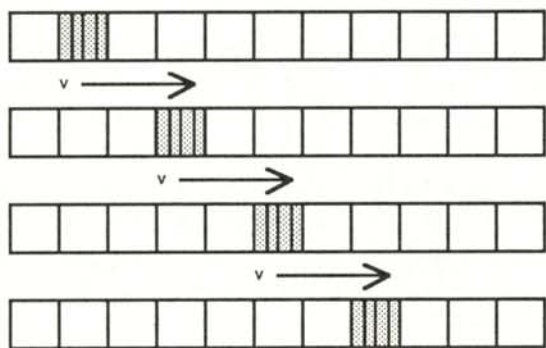


FIGURE 1

Schematic picture of the longitudinal sound wave

crease.

The effect of the moving medium on the velocity of sound was measured by sending a sharp sound pulse down a tube and measuring the time it took to travel this distance. An interface was built such that the experiment could be controlled by a Commodore C64 computer which would also calculate the value of the speed of sound. The system was calibrated by using for the speed of sound in still air a value calculated from the equation:

$$331 \text{ m/s} + 0.6 T \tag{1}$$

where T is the temperature in Celsius.¹

EXPERIMENTAL EQUIPMENT

A paper tube, shown in Figure 2, provided the control environment for this experiment. A Sears Shop Vac, used in reverse, provided the

the tube. When a sound pulse was detected, the crossing detector toggles the JK and this action puts a 0 on the Q output, thus closing the gate for the clock to pulse through. The JK cannot be toggled again because a 0 on Q causes a 0 on J and takes the 7476 out of its toggling mode.

The clock pulses were generated by 555 timers because of their clean symmetric waveforms and ease of operation. Since the C-64 I/O user ports are normally high², an inverter was used to flip this logic. The second transistor was used to increase the current flow from the inverter in order to power the second 555 chip.

PROCEDURE

The various potentiometers required adjustments for the first run. P4 and P5 (see Figure 3) must be adjusted to obtain clean and symmetric pulses from the output of 555#2. The pulses should appear as those in Figure 4. The audio frequency range was chosen so that the pulse from the speaker could be heard. P2 and P3 were ad-

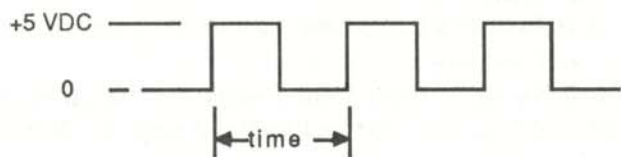


Figure 4

Shape of the pulses that are produced by the 555 timer. The potentiometers should be adjust to make the pulses symmetric.

justed until timer 555#1 produced pulses that were approximately 4 μs long. The exact time for one pulse was then recorded. The crossing detector's potentiometer, P1, was adjusted until the reference voltage from P1 was higher than the static noise voltage produced by the air mover. The speaker was pulsed to make sure that the sound would be detected and reflection problems avoided.

The operating program (see Table 2) was loaded and run. The C-64 counted the pulses that were

allowed through by the JK flip-flop. The computer multiplied the counts by the clock time and divided this into the distance between the speaker and the microphone. The speed was calculated by:

$$\text{Speed of Sound} = \text{distance/time} \quad (3)$$

The computer control gave the advantage of running many consecutive trials to measure the speed. The average of a multitude of trials with relatively consistent values assured that the errors were reduced in the measurements of the speed of sound. The results of the measurements in moving air are shown in Table 1.

Wind Speed	Speed of Sound m/s		
	Trial #1	Trial #2	Trial #3
0.00	346.29	346.44	346.48
3.35	347.00	347.40	347.38
5.55	347.22	347.85	347.89
7.49	347.80	348.54	348.41
9.26	348.40	348.93	348.19
11.2	348.80	349.51	349.79
12.0	349.80	350.00	350.27

TABLE 1

Summary of Data from the experiment. Notice the consistency of the results and any given wind speed.

CONCLUSION

There was one problem that arose in the experiment: the air mover produced static noise that was greater than the audio signal from the speaker. Foam insulation was placed inside the Shop Vac to muffle the static noise. A 15 turn potentiometer had to be installed at P1 to be able to set the crossing level properly. This seemed to solve the static noise problems, but care should be taken to choose the most quiet source of wind production available.

A curve was fit to the data using a Least Squares Fit routine and the following equation was found:

$$\text{Speed of Sound} = \text{SASS} + 0.3 W \quad (2)$$

where SASS is the speed of sound in still air and W is the wind speed. The still air average speed that we measured varied from that predicted by Equation 1 by 0.12%.

No straight forward relationship could be found in the literature between wind speed and the speed of sound. The empirical relationship of Equation 2 relates the wind speed and still air sound speed for the humidity, pressure and temperature conditions in the laboratory.

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2. Commodore 64 Programmer's Reference Guide, Commodore Business Machines, Inc., 1983 .

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```

10 Rem Measures the SPEED OF SOUND
20 Rem Written by:BILL RUSSELL
30 Rem   date: 06-14-87
40 Rem   for: SAU PHYSICS DEPARTMENT
50 Print <CLR>:Print:Print
60 Print "Input the distance from the speaker to
   the microphone in METERS"
70 Input D
80 Print
90 Print "Time for one clock cycle in SECONDS"
100 Input C
110 Print
120 Print "How many times do you want to run?"
130 Print"ZERO TO QUIT"
140 Input T : If T = 0 Goto 999
150 Print <CLR>:Print "Counts  Seconds  Velocity"
160 Print:
170 AV = 0
180 For x = 1 to T
190 Poke 56579,127:Poke56579,0:Rem sets
   JK
200 Poke 56590,16:Poke 56591,16:Rem Sets
   Up Counters
210 Poke 56591,65:Poke 56590,33:Rem Sets
   Up Counters
220 Poke 56579,128:Rem Beeps the Speaker
230 For Q = 1 to 50:Next Q:Poke 56579,0:Rem
   Gives Time
240 D1=255-Peek(56580)+255*(255-
   Peek(56580 + 1))
250 D2=255-Peek(56582)+255*(255-
   Peek(56582 +1))
260 CT=65025 * D2 + D1
270 SE=CT*C : MS=D/SE
280 Print CT;:Print" ";SE;:Print " ";MS
290 AV=AV+MS
300 Next X
310 AV1=AV/T:Print AV1
320 Print:Print:Print
330 Goto 120
999End

```

Table 2

Listing of the program used to operate the experiment

SCIENTIFIC WORK OF EVA VON BAHR

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ABSTRACT

At a time (the early 1900's) when women were still not generally accepted in the field of science, Eva von Bahr was conducting formidable physics research in such areas as the absorption spectra of gases, decomposition of ozone by ultra-violet rays and the absorption spectrum of water-vapor. Her life and work remain obscure despite their importance. This paper offers insight into Eva von Bahr's previously unrecognized scientific work.

INTRODUCTION

It is an unfortunate, but common enough practice for the works of some of the greatest scientific minds to be overlooked. The early 1900's, especially the years between 1905 and 1920, held a large collection of gifted scientists whose work was to have a profound effect upon the future. Germany, Austria and Sweden proved to be exceptionally wealthy in their share of the great minds during this period. A particular injustice was done to the women scientists of the era, some of whose contributions remain little known, even in the present. Lise Meitner is an excellent example of genius gone unnoticed. Other women included the anatomist Adele Hartmann, the archaeologist Margarete Bieber, the physicist Eva von Bahr and the mathematician Emmy Noether. All of their works have been largely neglected.¹ The intent of this study is to bring to light the works of Eva von Bahr, the German physicist. Dr. von Bahr is a case in point of women scientists whose discoveries were overlooked.

It is probably safe to assume that most of the readers of this paper have not heard of Eva von Bahr. To provide an introduction to the contributions of Dr. von Bahr, a section of her research, conducted between the years 1907 and 1914, has

been selected for examination.

Several of her works appeared as communications from Uppsala University in Sweden. It was there that she was a Privatdozent², which is an unsalaried lecturer, a relatively unusual position for a woman to attain at that time. Uppsala University had a long and impressive history. It was founded in 1477, and could boast a number of prominent scientists by 1900. These included: Jons Jacob Berzelius, Svante Arrhenius, Anders Jonas Angstrom, Manne Siegbahn and numerous others.³ It has been said that these represent the "values common to the scientific spirit of the twentieth century."⁴ These values were perhaps intensified because the scientists came from a small country and felt that they had to reach an especially high level of excellence in order to obtain international recognition.

ABSORPTION EXPERIMENTS

In 1907, Eva von Bahr was conducting research on absorption of radiation by ozone. In her publication of the work, she provided measurements of the absorptive power of ozone for thermal radiation from sources at different temperatures. Her sources for the experiment were black bodies at -70 C, 216 C, 352 C and a Nernst

Lamp. The heat measurements were made with a bolometer, invented in 1880 by S.P. Langley. The ozone measurements in this experiment were done with two parallel glass tubes with rock-salt ends. The tubes were filled with pure oxygen and were connected together through a sulphuric acid manometer. Figure 1 shows a diagram of this equipment.⁵ The oxygen in one of the tubes was ionized by the passage of a 'silent discharge', and the fall of pressure then indicated the amount of ozone formed.⁶

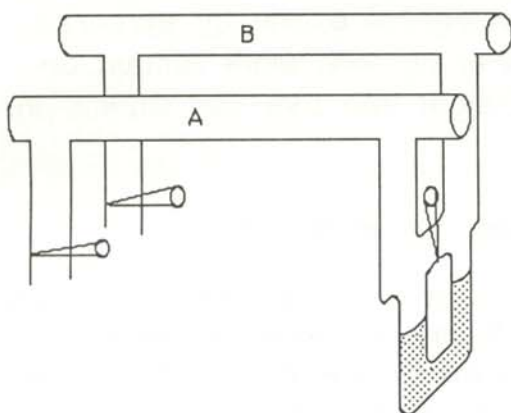


Figure 1

Equipment used to study the absorption of thermal radiation by Ozone.

Another publication appeared in July, 1909. This research was a continuation of Angstrom's work (1901) and dealt with the influence of pressure on the absorption by gases of infra-red rays. Angstrom found that the absorption of infra-red rays by a gas depends upon the total pressure. The original work was done for CO_2 . In this experiment, the absorption by a fixed quantity of CO_2 was measured. The gas was then allowed to expand and absorption was measured at the lower pressure. This absorption turned out to be less than the first. An inactive gas was then admitted until the initial pressure was restored, at which time the original value of the absorption

was observed. Eva von Bahr then extended these observations to other gases: CO , CH_4 , C_2H_4 , N_2O and NH_3 . The same results were obtained with all these gases. With methyl and ethyl ethers, however, the absorption for the lowest pressure was somewhat less, but the difference was so small that it fell into the margin of error.⁷

In September, 1910, Eva von Bahr published more results of her research. The influence of increased pressure on the absorption of infra-red rays by gases was her topic. She found that the absorption increased in general when the gas pressure was increased by adding another gas. However, the maximum absorption was reached at different pressures in different gas mixtures. From her results, specifically from comparisons of her 'pressure curves', it seemed to her that a gas that had large molecules obtained its maximum absorptive power at lower pressures than a gas with small molecules. Another part of her research published at the same time included work on the decomposition of ozone by ultra-violet rays. As we know, she had already shown that the absorption of infra-red rays by ozone increased with increased pressure. One could expect a similar increase of absorption of ultra-violet by ozone. The ultra-violet rays were found to have a strong de-ozoning effect. This de-ozoning became more noticeable as the pressure was lowered. It seemed to be due to rays of wavelength ranging from 230 to 290 μm .⁸ In 1911, Gustav Hertz extended the work of von Bahr and Angstrom. Their results were confirmed.⁹

The influence of temperature on the infra-red absorption of different gases was published in 1912. In her previous work, von Bahr found that infra-red absorption by gases depends upon the pressure. In this particular work, she showed that the effect of temperature on the infra-red absorption is very different from that of pressure. Increases in temperature seemed to have an effect on the absorbing particles themselves, while an increase of pressure to a certain extent,

increased the number of these particles. The temperature effects were tested using CO_2 , CO , N_2O , CH_4 and other vapors. ¹⁰

In August, 1913, the effect of pressure on the absorption of infra-red radiation in gases was again reported. This research investigated the relation of the pressure and absorption of waves from 100 to 350 μm in HCL , SO_2 and H_2S . ¹¹

She continued her research on absorption by gases of infra-red and in particular the absorption spectrum of water-vapor. She found that the absorption bands of gases were discontinuous at low pressures. The discontinuities, however, were less evident as the pressure increased. The bands, where the maximum absorption was obtained, appeared to be almost continuous. ¹² She concluded that the absorption bands of water-vapor probably constituted a Bjerrum double band. In 1912, Niels Bjerrum, in what turned out to be a very important paper, discussed his research on the structure of bands of the infra-red absorption spectrum. He thus dealt with the problems of quantization of rotational energy. ¹³ Both parts of the Bjerrum double band appeared to be made up of a large number of narrow bands. ¹⁴ Dr. von Bahr continued this type of research with HCL and CO_2 through November, 1913. With these experiments, she demonstrated that the Bjerrum concept of the far-infra-red absorption spectra of gases was in agreement in many ways with the experimental results. ¹⁵

IONIZATION POTENTIAL EXPERIMENTS

At the beginning of 1914, Eva von Bahr and James Franck published the results of their work together on the ionization potential of positive ions. Their research was an attempt to determine the minimum voltage at which positive ions can become ionizing agents. An incandescent platinum wire was used as a source of the ions. It lay along the axis of a cylindrical platinum cage. The positive ions were sent by means of an applied electric field through the surrounding cage into a

ring-shaped space beyond, where they encountered a reverse field which sent them back to the cage. The ionization produced in the ring-shaped space was measured by the current of negative ions passing through that space to an outer platinum cylinder.

The results show that under the conditions of the experiment, positive ions are much less effective ionizing agents than electrons. No definite minimum ionization voltage could be determined from the data. ¹⁶ Franck and von Bahr each became involved in other research, and so did not continue their work together. The experiment, however, provided a background for Franck and Gustav Hertz when they conducted their now famous Franck-Hertz experiment.

MOLECULAR ROTATION EXPERIMENTS

Dr. von Bahr returned to her work with infra-red radiation. She had become much more sophisticated, and now dealt with molecular rotation and the photon hypothesis. In 1913, Max Planck had proposed Albert Einstein for membership in the Prussian Academy, and was quoted as saying:

"That he may sometimes have missed the target in his speculations, as for example, in his hypothesis of light quanta (photons), cannot really be held against him, for it is not possible to introduce fundamentally new ideas, even in the most exact sciences, without occasionally taking a risk." ¹⁷

It is evident from this quotation that even Planck was unwilling to accept Einstein's light quantum hypothesis. Indeed, photons were not generally accepted as real entities until the early 1920's. Regardless of this, just one year after Planck made the statement, Eva von Bahr was among the first to employ Einstein's photon hypothesis in her research dealing with molecular rotation. ¹⁸ This was in Dr. von Bahr's publication of July, 1914 and was titled, "Molecular Rotation Energy and the Quantum Theory." ¹⁹

In 1938, Eva von Bahr allowed her friend Lise Meitner to stay with her following the latter's escape from Nazi Germany. In her 1938 correspondence with Otto Hahn, Meitner mentions her intentions to go and stay with Eva von Bahr-Bergius (she was married by this time) in Kungälv, Sweden.²⁰ There is no mention of any research Dr. von Bahr may have been conducting at that time.

This paper was meant to serve as a very general introduction to Eva von Bahr through some of her works. She was unfortunately a 'victim' of her time period. She is one among many women of the early 1900's whose works and efforts may never be fully recognized.

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AN ANALYSIS OF TWO COLOR DIAGRAMS FOR NORTHERN CEPHEIDS

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ABSTRACT

The slopes of the two-color curves for 45 cepheid stars are analyzed. The relationship between the slope and the luminosity period is perceived, and an astrophysical relation proposed. The sample group contains both binary and single cepheids.

INTRODUCTION

The two-color diagram is a plot of the U-B versus B-V, where U, B and V are color indices that rate the intensity of an object's light in the Ultraviolet, Blue and Visible (Yellow) spectra. It is a commonly used tool in understanding a type of star known as a cepheid, because cepheids are variable stars, whose luminosity, temperature, radius, radial velocity and surface gravity change with time. These changes can be correlated with fluctuations in both the U-B and B-V indices. In particular, the U-B index is a strong function of surface gravity. The B-V index is a strong function of the effective or surface temperature due to the location of the peak and the shape of the continuous spectrum with respect to the U, B and V wavelengths.

Cepheid variables are thought to be stars undergoing core helium burning, stars nearing the end of their life cycles. This helium fusion at the hydrogen depleted core of the star disturbs the generally homogeneous structure of the star. It sets up shells of ionized hydrogen and helium, whose heat capacity and absorption characteristics are such that they generate pulsation in the outer layers of the star.

Cepheids are distinguished from among the

many classes of variable stars because of the highly regular periodicity of their pulsations and their relative abundance. The majority of stars pass through a cepheid phase during their evolution. A regular relationship has been found between the absolute magnitude (or total output of a cepheid and the period of its pulsations. When combined with the absolute/apparent magnitude relations, it gives a decent estimate for the distance of any given cepheid, based on the easily determined period of its pulsation and apparent magnitude. ^{2,3}

The next step is to use cepheids, which tend to be quite bright, as yard sticks. This is now one of the most trusted distance determiners, and, in fact, is one of the major stepping stones to determining cosmological distances. So, any greater understanding of the nature and mechanics of the cepheid variable is of great interest to contemporary astronomy.

TWO-COLOR DIAGRAM SLOPE

As time passes, an individual cepheid should trace out a loop on the two-color diagram. This loop may then be analyzed to determine certain characteristics of the system. This has been done for a cepheid in the presence of a companion. ¹

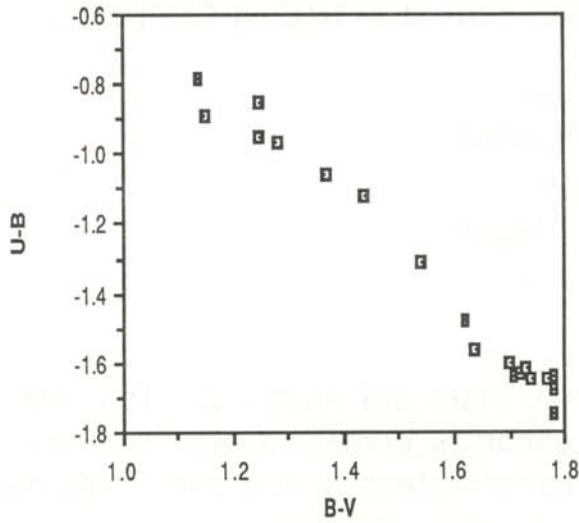


Figure 1
Two color diagram for the single cepheid SV Vulpeculae⁶

But in practice, with average quality photoelectric photometry, the cepheid covers at best a well defined blob on the two color diagram. This type of data defies chronological analysis and lends itself to a general determination of the slope of the

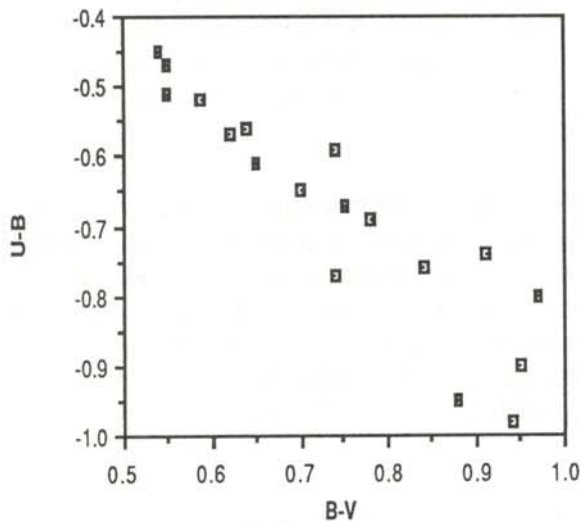


Figure 2
Two color diagram for a single cepheid TX Delphini⁵

cepheid's average motion on the two-color diagram.

Three examples are given in Figures 1, 2 and 3. They illustrate the range of the shapes encountered in two color diagrams.^{4,5,6} All three diagrams are of single cepheids, and yet only Figure 1, SV Vulpeculae, has the "tight loop" format commonly associated with single cepheids. TX Delphini (see Figure 2) exhibits an interesting "flare" format. SU Cassiopeiae (see Figure 3) has a definite broad format, suggesting a binary companion, yet none has been observed.

PERIOD VERSUS SLOPE

Figure 4 shows a plot of the two-color diagram

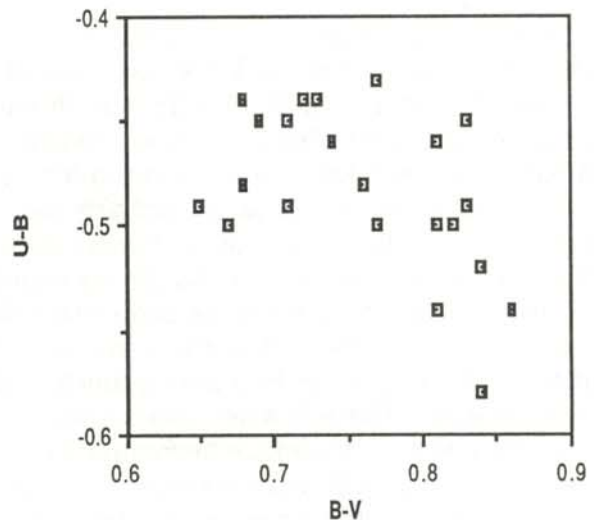


Figure 3
Two color diagram for the single cepheid SU Cassiopeiae⁴

slope vs. the log of the period. It reveals a definite relation between slope and period. The two anomalous points are DL Cas, whose brightness in ultraviolet is too low for accurate photometry, and RW Cam, whose diagram is highly dispersed by its binary companion. The known binary systems are indicated. Except for the extreme case of

RW Cam, they appear in proportion and follow the downward trend. 7

DISCUSSION

The general relationship between changes in luminosity (L) and corresponding changes in stellar radius (R) and effective or surface temperature (T) is given by the Stefan-Boltzmann equation:

$$\Delta L \approx L(2/R \Delta R + 4/T \Delta T) \tag{1}$$

This, combined with the surface gravity identity:

$$\Delta g \approx - M/R^3 \Delta R \tag{2}$$

where M is the mass and g the surface gravity, produces an equation relating luminosity changes to surface gravity and temperature changes:

$$\Delta L \approx L(C_1 R^2 \Delta g + C_2/T \Delta T) \tag{3}$$

where C₁ and C₂ are constants.

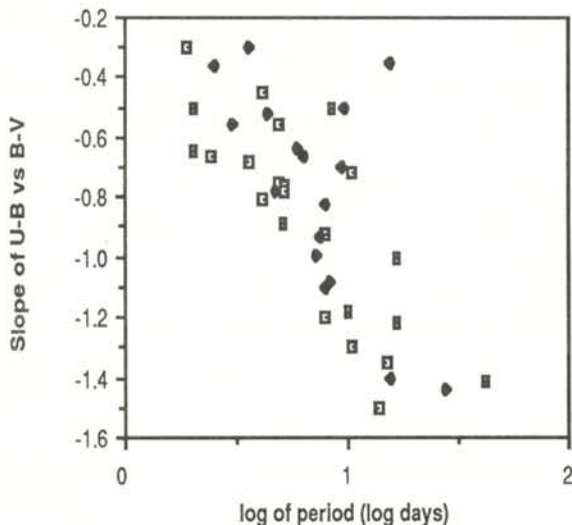


Figure 4

Plot of the two color diagram slope versus the log of the period for 45 northern cepheids. The binary systems are the solid squares. 4,5,6,7

Equation 3 implies that changes in the luminosity of a star are closely tied to the ratio of changes in its surface gravity (effectively the radius) and temperature. Figure 4 shows a proportional increase in surface gravity with increasing period. The slope of a U-B vs B-V graph becomes more negative as the period increases. In two color diagram terms, this steeper slope, indicates a greater surface gravity contribution.

This empirical proof of the surface gravity/temperature ratio to period connection deserves further study. It should be especially valuable with a quantitative analysis of how radius and temperature changes effect the period of oscillation of the Cepheids.

ACKNOWLEDGMENTS

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POST USE BOOK REVIEW*GENERAL PHYSICS* by Douglas C. Giancoli

Prentice Hall, Inc., Englewood Cliffs, NJ 07632 1984

Reviewed by:

Jeff Blackmon, Guilford College, Greensboro, NC 27410

Giancoli's *GENERAL PHYSICS* was my first physics textbook. It at first struck me as being both expensive and difficult, but as I have continued on in physics, I have realized that Giancoli is neither. Giancoli makes an honest but faltering attempt to add freshness to the almost nine hundred pages of his text.

The text suffers from being too conservative. The bulk of the book is mechanics. Giancoli argues that since it was developed first, and is the basis of so much other physics, it should be studied first. But despite the simplicity with which Giancoli tries to present it, the student would be far better off with a semester of Calculus before starting on mechanics.

The chapter on special relativity (Chapter 39) would be a good way to start a course. It is interesting to students; no calculus is involved, and it deals with measurement - fundamental to physics. But even though *GENERAL PHYSICS* is set up as to allow the professor some flexibility in the order of presentation of material, the chapter on special relativity presupposes other physical concepts introduced in the mechanics chapters. Waves could also be a better beginning topic for this book, giving students some basic understanding of the elementary concepts in physics without bogging them down with calculus or avoiding it.

Giancoli does a good job with the chapters on mechanics. His introductions of 'instantaneity'

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and subsequently calculus are clear, but not much different from those in a standard calculus textbook. He falters in the chapter on 'Kinematics in 2 and 3 Dimensions' (Chapter 3) with his presentation of vectors. He presents too much vector math without physical examples, defining terms and presenting methods without presenting arguments of why they make sense. He ultimately does the same thing with both the dot and cross product, giving the students no intuition into the concepts.

Circular motion is introduced in Chapter 5 with classical examples (such as the ball twirling on the end of a string), but he does succeed in getting his points across clearly and concisely. In Chapter 9, Giancoli does an excellent job with rotational motion. The student would be helped with more 'hands on' examples, especially with an air table. An example of an excellent section is the one titled 'Why Does a Rolling Sphere Slow Down?' (9-7), which gives the student good insight into a not so straight forward problem.

The introduction to waves (Chapter 15) is average, not much different from any other I have seen. The same is true of his treatment of thermodynamics. The chapter on kinetic theory (chapter 18) is very abstract, but if the student survives, it is followed by a very clear and intuitive chapter on heat. Electricity and Magnetism is also not treated in a new or exciting way. Some of the explanations are quite clear, while others are somewhat awkward. They seem to cancel each other out, making *GENERAL PHYSICS* average.

The problem sets in *GENERAL PHYSICS* are good throughout. The problems are of a wide range of difficulty and approach. The professor

has work to do in selecting an appropriate problem set, but one can be found for almost any range of freshman students. Giancoli does try to incorporate numerical methods when first introducing the integral. Numerical methods still do not get the attention that they deserve, nor is their importance emphasized. However, Giancoli does at least give the student some introduction to them. Also, the tables of constants and units on the inside cover are excellent. They contain most of the information students frequently need to look up, but not a great deal of unnecessary data. Also impressive is the printing of the book. There are relatively few errors in the problems and solutions. This is not my usual experience with the first edition of a text.

One other drawback of Giancoli is the appendices. Of the four included, only the unit on polar coordinates is of any merit, and, to say the least, is skimpy. The mathematical formulas appendix (A) is somewhat useful, but not thorough enough to be a great consequence. The calculus appendix (B) is only confusing. Appendices are a good tool to give students background they need and may not have and to touch on concepts, the scope of which are beyond the realm of the book. Giancoli only uses them as tables of information he feels students may need to look up.

Giancoli is a good freshman text. The writing style is simple, often presenting material in a fresh dialogue, and not often convoluted or unclear. The problem sets are good, but must be sorted properly by the professor. The overall approach, however, is not new. The book loses much of the freshness of writing with inadequate examples and references, leaving Giancoli a good, but not great, lower level freshman text.