**Numerical Solution to Transient Heat Flow Problems**

Ronald A. Kobiske, and Jeffrey L. Hock

Citation: American Journal of Physics **41**, 517 (1973); doi: 10.1119/1.1987281 View online: https://doi.org/10.1119/1.1987281 View Table of Contents: https://aapt.scitation.org/toc/ajp/41/4 Published by the American Association of Physics Teachers

**ARTICLES YOU MAY BE INTERESTED IN**

Nonrelativistic contribution to Mercury’s perihelion precession American Journal of Physics **47**, 531 (1979); https://doi.org/10.1119/1.11779

The harmonic oscillator at finite temperature using path integrals American Journal of Physics **56**, 1129 (1988); https://doi.org/10.1119/1.15737

Path integral for the quantum harmonic oscillator using elementary methods American Journal of Physics **66**, 537 (1998); https://doi.org/10.1119/1.18896

Classical Limit of the Hydrogen Atom American Journal of Physics **41**, 525 (1973); https://doi.org/10.1119/1.1987282

A simple numerical model to simulate a gas in a constant gravitational field American Journal of Physics **68**, 61 (2000); https://doi.org/10.1119/1.19374

Solutions of Kronig-Penney Models by the T-Matrix Method American Journal of Physics **41**, 512 (1973); https://doi.org/10.1119/1.1987280

*April 1978*

**Numerical Solution to Transient Heat Flow Problems**

RONALD A. KOBISKE JEFFREY L. HOCK *Department of Physics Milwaukee School of Engineering Milwauke*e, Wi*sconsin 53201 (*Received 24 June 1972; revised 27 September 1972)

We *first consider the partial differential equation that governs one-dimensional heat flow in a homogeneous medium. This equation is reduced to a difference equation*

*and the problem of difference equation stability and con- vergence is discussed and examples of the breakdown of each are given. Next, the above analysis is extended to a three-dimensional space with spherical symmetry. Several interesting problems are programmed and the solutions are displayed in graphical form. The accuracy of the numerical difference technique is checked by comparison with exact Fourier series solutions. The paper is mainly intended for beginning students of physics and engineering, and also for college teachers who have not had a formal course in numerical solutions of partial differential equations.*

under conditions where certain boundary condi tions change with time in a periodic manner. Examples of this phenomenon are evident in the cylinders of internal combustion engines, on industrial processes where thermal cycling of a system occurs, and in space applications where an instrument package is subjected to wide periodical variations in temperature.

For many beginning students of physics and engineering, the subject of numerical analysis could encompass a broader range of topics than it usually does. If they take a course in numerical analysis, all too often they only program solutions to simple ordinary differential equations. A typical problem being that of the calculation of the path of a projectile in flight. If we think about it, we will realize that most physical phenomena are describable by some partial differential equation or collection of such equations. Our purpose in this paper is to discuss a simple method for programming solutions to the partial differential equation that describes diffusion processes. We display several interesting physical problems, their solutions, and discuss the physical sig nificance of the solution.

Having carried through a solution to an equation of this type, students will be in a better position to appreciate the roll that such equations play in describing the physical phenomena in the world around them.

**I. INTRODUCTION**

In our everyday experiences we are all familia**r II. THE DIFFUSION EQUATION AN*D* A** with the process of diffusion. A drop of black in**k DIFFERENCE COUN*TE*RPART** will diffuse when placed in a container of water;

**A. The One-Dimensional Diffusion Equation** heat will diffuse toward your hand when you hold - a metal bar in a flame. Other diffusion phenomena The general form for the diffusion equation in a include neutron diffusion in the moderator around homogeneous medium is given as:1 a reactor or neturon source, diffusion current is very important in a consideration of moving

Q2*727=0T/at* charge carriers in semi-conductor devices, and introduction of impurity atoms into solids by a where *T,* for the problems considered in this diffusion process is important in the area of paper, will represent temperature in degrees electronic devices. In many cases of practical Celsius, *t* represents time in seconds, and a is interest, diffusion conduction processes occur the diffusivity with units of cm/sec1/2. One can

(1)

*AJP Volume 41*

*517*

R*. A. Kobiske and J. L. Hock*

mated by the following expression:

TEMP.)

**T(m+,n)**

Tim,n)

**| Tm+1,nh-mn)**

- - - - --

-

-

*32T/8x2 =* 2 (slope) */ox*

=[(slope)2-(slope).]*/h.* This yields:

T(m,n)-T(m--1,n)

- --

Tím-1,n) ---

1

-- - - -- - Thaith

**x(m–1)**

**x(m)**

**x(**m+1)

*22T/0*x2=[*T(m*+1, n) *+T(m-*1, n)

*-2T*(*m, n*)]*/h*? (3)

FIG. 1. A general curve of temperature vs linear distance for a particular time *t*.

Similarly, a finite difference form of *aT/at* is:

*OT/at*

*[T(m*, n+1)-*T(m, n*)]/A.

(4)

show that a’ is related to certain material param eters of the medium by:? a?*=k/pc*, where k is the thermal conductivity, p is the material density, and c is the specific heat capacity.

In one dimension, V2 has the form *02/a*xo. Thus, in this representation, Eq. (1) becomes:

Substitution of these approximations into Eq. (2) yields the following difference equation:

*T(m*, n+1)*=T(m, n*) +*(a’At/ha)*

X[*T(m*+1, n) +*T(m*-1, n)-*2T (m, n*)). (5)

q?*32T/8x2 = ƏT/at.*

It is this equation, which in some cases will contain additional terms, which describes the various diffusion processes that were discussed in our introduction. The derivation of this equation is adequately covered in Sears, and also in many other general physics texts. Since its inclusion here would add nothing new, we will omit this con **sideration.**

Solution to this equation gives the temperature at point x(*m*) for so**me advanced tim**e *tn*+1) in **term**s of what it was at point \**(m-*1), x*(m),* and x*(m*+1) for some previous time *t(n*). Thus, if a temperature distribution is given for all positions at *t*=0, and for all times at t=0 and *x=L*, one can map the time evolution of the system from the difference Eq. (5).

**B. The Difference Equation**

Consider a solid of length *L. W*e represent this distance by an integer number of equal sub intervals of length h. Thus, a general distance is *x =mh* and is represented by the notation x*(m*), where *m* is an integer. In the same way, we quantize the time according t*o tn*a*t*, and apply the notation *t(*n). The temperature at position x*(m*) and time*t(*n) will be represented by *T(m,n).*

The difference equation will be derived under the assumption that the slope of the temperature distribution can be considered constant over the spacial interval *x(m*) to x*(m* +-1). Referring to Fig. 1, two successive slopes are:

**C. Errors**

It turns out that the above difference equation does not describe the actual physical situation for all values of *B=Ataạ/h*aWhat we have essentially done was to convert a partial differential equation, which represented the exact situation at all points, to a finite difference equation that con sidered only a small finite number of points. This greatly simplified pi**cture immediately raises** questions on how well can one expect to describe the situation, what time jump to use, and what might be a good choice on cell spacing? What sort of round off error, associated with the way that a computer does its computation, can one expect*?* For certain values of the parameter *B*, the solution to the finite difference Eq. (5) diverges or oscillates about the true solution that is described by the differential Eq. (2). Following G. O'Brien, let *D* represent the exact solution of the partial differential Eq. (2), and A the exact solution of the

(slope)a=[*T(m*+1, *n*)*-T(m, n)]/h,* (slope)1=[*T(m, n)-T(m*-1, n*)*]*/h.*

In a finite difference form*, 32T/a*x2 can be approxi-

*518 / April 1973*

*Numerical Solution to Heat Flow Problems*

TABLE I. Convergence and stability are shown for a'A*t/h2*-1 in the difference equation

*T(m*, n+1)=*T(m,* n) +(aA*t/h2) [T* (m+1, n) +*T(m*-1, n*) –2T (m,* n)].

*n m*o

1

**0**

**1**

**Halos**

1(c)

*(*5*/*8) (te)

*(7/8) (d*e)

*(*5/8)(te)

O

*(17/*32) (te)

(3*/*4)(3€/8)

*(1*7/32) (te)

lo

(29*/*64) *(76/*32)

(41/64) (5€*/*16)

(29/64) *(*7*/*32)

0

To

(99/256) (12€/64)

(140/256) *(1*7/64)

(99*/*256) (12€/64)

0

partial finite difference Eq. (5). Let *N* represent for the two values of the B parameter. For the the numerical solution of the partial difference moment, ignore the numbers in the brackets. equation. *(D*-A) is called the truncation error; In Table I it is not difficult to believe that, even it arises because of the finite distance between though the values obtained for any give*n h* are points of the difference mesh. To find the condi- not smooth, the numbers obtained by this process **ti**ons under which A*D* is the problem of con- would approach the exact solution of the partial **vergen**ce. *(*A-*N*) is called the numerical error; differential equation as *h* and A*t* were decreased. in our discussion it is limited to round off error. In Table II the solution is in a state of oscillation; To find the conditions under which *(*4--*N*) it would be very difficult to believe that this **remains sma**ll as time advances is the problem of solution could represent the exact solution. We stability. In order to illustrate the dependence of would say that the solution of Table I is convergent **convergen**ce*/*stability upon the parameter *B*= while that of Table II is divergent. In order to *a’At/h2,* we will introduce the following example: study the stability let us introduce a numerical

Let *T*(x, 0)=1 for 0<x<1, *T(0*, 1) =0, error e at *T(*2, 1) and follow this error as it *T(1*, *t*) =0, with B-1, \, an*d h=1*. In the matrix propagates. In Table I the error decays, while in tables that are displayed in Table I and Table II, Table II, the error oscillates in sign and grows as we show the numerical solutions to this problem time is advanced. We would say that the solution

Table II. The breakdown of both convergence and stability is shown for *a'At/h*2= 4 in the difference equation

*T(m, n*+1)=*T(m,* n) +*(a?At/h2) [T(m* +1, *n)* +*T(m*-1, n) - *2T (m,* n)].

*n*i mlo

**1**

**2**

1(c)

**()**

*(*5/*8)* (3*/4)*

-*(1/*8) (-- de*)*

*(*5*/*8) (3*/*4)

- (13/32)(-30*/4*)

1(11:/8)

- (13*/*32) ( -- 3/4*)*

(61/64) (45€/32)

*-(71/*64) (-29€16)

(61/64) (45€/32)

0

5

10

– (335/256) (-132€/64)

(294*/*128) (193e/64)

-(335*/*256) (-132€/**64)**

**0**

A*JP Volume 41 / 519*

*R. A. Kobiske and J. L. Hock*

t=0

insures both stability and convergence of the difference equation.

**T=15.15ec.**

**III. A ONE DI*M*ENSIONAL HEAT FLOW PROBLEM**

t=30.2

***M*P**

Consider a rectangular piece of copper of length **t=45,3**

*L,* with insulated sides, ends held at 0°C, and an T=60.4 Sec

initial temperature distribution given by: \_T:*75*5

*T(m*, 0) = 100°C, *m+*0, *L/h;* **10 12 14 16 18 2*0* LENGTH IN CM**

*T(*0*,* n) *=T(L/h, n)* =0°C. FIG. 2. Temperature distributi**ons in a rectangular copper bar.**

The difference Eq. *(*5) **was programmed** (See Appendix A) for this problem and the

**numerica**l results are displayed in Fig. 2. In order of Table I is stable while that of Table II is to have an integer number of spatial divisions **unsta**ble. One can show that' the error e obeys the between zero and *L*, it is convenient to choos*e h* **same difference equation as the temperatur**e and allow the stability relationship shown in Eg. distribution A*(m, n)*. This is important in that it (6) to determine *At.* **indicates that € and** the transient part of A*m, n)* The previously defined constant, a’, has the **usually have the same growth properties. The** value of 1.10407 cm2/sec, for copper.2 The value of word "usually” was used rather than “invarably," *L* was chosen to be 20 cm*, b*=1, and *h=*1 cm. This **becau**se one must consider the effect of **an initia**l produces a time step of *At*=0.150956 sec. condition which influences A*(m, n*) but not the In Appendix B an exact Fourier series solution **error e.**

to the above problem is given. This series is It can be shown that a stable solution results summed to insure a con*v*ergence to six significant f*o*r *B*< . Thus, *B*= separates the region of digits for the times displayed in Fig. 2. The **stab**ility, where e**rrors decay, from the region o**f results of a numerical comparison of the above **insta**bility, where errors grow. In order to establish methods indicate a maximum deviation of 0.36%. **some criterion for convergence, we again referen**ce The result of this comparison also indicates that O'Brien. Consider the same problem that we the above numerical technique is stable and **employ**ed to distinguished **between convergence converg**ent. This gives one confidence that the and stability, O'Brien has given an exact solution application of this technique to more difficult, to our difference Eq. (5) for this problem: not so easily checked, problems will yield reliable

**results.**

The basic diffusion mechanism is very easy to see and understand in this problem. Heat simply diffuses out of the bar through the ends, which are maintained at a fixed temperature. The final steady state temperature is that of the ends. An

interesting extension of this problem might be to where: *x=j/M, t=k*a*t, b=a+At/ha,* and M repre- consider the ends held at different temperatures. sents the number of cell spacings.

The final steady state temperature distribution is As time increases, *k* increases, and for the last already familiar to students who have had a first factor to remain finite, *ß* must be less than or course in Physics and is simply a linear distribution equal to 1.

between the end poi**nt temperatures.** Thus, the choice of:

A more interesting situation arises if we con

sider two materials with equal thermal conduc *B*=*a'*A*t/h? <)*

(6) tivities k, but with different densities p and heat

***M***

**-1**

***j*=1,3,5**

*T(*e,t) - À 2 cot (3)

X sin (Ija) [1–48 sino ()

*520 ) April 1973*

*Numerical Solution to Heat Flow Problems*

capacities, Cy. From general physics, one knows transformation: that the steady state heat current depends only upon the thermal conductivity; however, for the

*T(1, 1)* = V*(*r, *t)/r.* transient response, as the steady state is ap proached, the transient heat current also de- It is easy to show that if *T(*r,*t*) is a solution to pends upon both the material density and heat Eq. *(*7), V(r, *t*) is a solution to Eq. (2) with x capacity. Thus, the above materials will have replaced by r: identical steady state heat currents for equal b*o*undary conditions at the ends, but will have

*a*%a2V *(*r*, t)/ap2 -*= a V (1*,)/at.* (8) much different transient responses in the decay toward the steady state. Students might expect, A difference counterpart for Eq. (8) has already from consideration of steady state heat flow, that been developed in Sec. II-B, Eq. *(*5), and is the termal conductivity alone will control the restated here using the transformed variable results rather than the density and heat capacity *(m, n*): in addition to the conductivity. Physically, the amount of heat stored per unit volume depends V(m, n+1) = V(*m*, n) +(*a*’*At/ha)* on the product of heat capacity and density; in a

X[V*(m*+1, n) +V(*m-*1, n)-2V*(m,* n)]. time changing situation, this storage consideration is important while, in steady state heat transfer all elments of mass have fixed amounts of energy.

Under the conditions of stability and convergence The heat current depends only upon the ability of [Lq: 10*)*. We have: the medium to transfer heat by the conductivity mechanism. Each element of mass acts as a source

*V(m, n*+1) = V(*m, n)* or a sink for the energy being transferred, while the

+[V(m+1, *n*) +V(*m-*1, *n)*], (9) energy associated with each element is held constant. In a consideration of transient flow, the

where a value of i has been choosen for the condition of constant energy per mass cell does parameter a *At/ha.* One advantage to using the not hold. In order to investigate this effect, a

above transformation is that the previously dis student might look up the material parameters of cussed error analysis can now be applied directly nickel steel (70% Ni) and also those of lead.

to this new three-dimensional problem. Thus, we The above problem could be programmed, and the can form a numerical solution to this new dif resulting transient temperature distributions com ferential equation by applying previously pared. After a little search, he will find that

developed techniques. Using the theory developed several other pairs of materials are also suitable to above we shall discuss the programming of a display the above effect.

practical problem.

**IV. A THREE-DIMENSIONAL HEAT FLOW PROBLEM WITH SPHERICAL SYM*M*ETR*Y***

**A. *A* Difference Technique for Spherically Symmetric Problems**

In this problem we extend the technique developed previously to three-dimensional space with spherical symmetry. In this spherical coordinate system the form of the diffusion equation is?:

**B. A Three-Dimensional Heat Flow Problem**

Consider the situation where a copper sphere of radius a is initially held at a constant temperature *To*. The surface of the sphere is then brought into contact with an ice bath of temperature 0°C. *W*e wish to plot the spatial temperature distribu tion for different values of time.

In the *T(r, t*) variable the initial conditions are:

*T(a, t*) =0°C, *T(*1,0) *=T,*= 100°C,

a?[*aT/8r*2+*(2/r) (aT/ar)*]=*aT/åt, (7)*

*1 ta*

where r represents a radial distance. Consider the

The problem now proceeds as in Sec. III. The

*AJP Volume 41 | 521*

***R. A. Kobiske an****d J. L. Hock*

conditions become:

**t=0**

V(a, *t)=aT,* sinut, V(0, *t*) = V(7,0)=0.

t=302 Sec.

**TE*M*P.**

t=906Şect

=60A

**t=120.8 t=151**

*Ž*

*o*

o 0 2 14

**RADIUS IN CM.**

16

18

*20*

22

*2*4

**Fi**g. 3. Temperature distributio**ns in a copper sphere.**

numerical results of this calculation are displayed in Fig. 3. The inverse transformation *T(*r, *t*) = V*(*r, *t)/*r has been used to transform all numerical data back to the *T(r, t*) representation. *T(*0, *1*) is found by making use of a three point inter polation scheme. An exact solution to this problem is displayed in Appendix B. The results of a **num**erical comparison of the difference technique with the exact solution are identical to those of the previous problem.

The condition V(0, *t*) =( must be imposed to insure that *T(*0,t) will be finite at r=0. As in the **previo**us section, *T*(0,*t*) will be found by using a three-point interpolation scheme.

Displayed in Fig. 4 are several temperature distributions which exhibit the time evolution of the system. The exact solution was obtained with the aid of Laplace transforms. For the interested reader, this solution is displayed in Appendix B. For comparison, to test the accuracy of the differ **ence schem**e, this series was summed to 2000 terms and compared with the results of the numerical difference technique. For this comparison, the **time was advan**ced to 200 sec. The results agreed to within 3%.

One can observe a steady build-up in tempera **ture at the cent**er of the sphere. **The remainder of** the system will continue to oscillate in temperature as the steady state is approached. The analytical solution to the problem is interesting in that, if one proceeds with a standard separation of vari able technique, with a real separation constant, **one cannot introd**uce the time changing boundary condition. One must introduce a complex separa tion constant and proceed from there. The equa tion that then results is a Schrödinger type equation which does admit oscillatory solutions. On the other hand, if one applies the method of Laplace transforms in a direct way the complex separation constant is hidden in the operational

**With**

**C. A Spherical Diffusion Problem Time-varying Boundary Conditions**

We shall now consider a problem which is analytically a more difficult problem than those considered so far. This problem will involve time changing boundary conditions.

Consider a sphere of radius "a" initially at a temperature of 0°C. Let the surface of the sphere be in contact with a source of heat which produces **a variation in surfa**ce temperature according to:

*T(a, t) =T*o sino*t.*

**t=30.2**

t=60.4 Sec.

t

õ

e too 72

to 18 20 22 24 50

***T*E*M*P**

**T=120.8**

Following the previous discussion, we **again wish to program th**e difference Eq. (5) subject to the above conditions. We take the form of the partial difference diffusion equation as that of Eq. (9), **where the transformatio**n V(r, *t)=rT(*r*, t*) has been applied. Recall, *T(m, n) c*orresponds to the **temperature di**stribution in the spherical space, and V*(m, n*) is the associated temperature dis tribution in the equivalent linear medium. Under this transformation the new boundary and initial

**á**

t=906 Sec

**-80**

**-1001**

RADIUS IN CM. FIG. 4. Temperature distributions in a copper is subject to sinusoidal surface t**emperature variations.**

***w*hich**

*522 / April 1978*

*Numerical Solution to Heat Flow Problems*

technique. The oscillatory behavior of this system the undergraduate physics and engineering is interesting from the standpoint that one does student. Three problems of increasing difficulty not usually associate a diffusion process with a were presented, and computer solutions were wave type of motion. While the situation that we graphically displayed. Exact series solutions were have discussed is not strictly wave motion, it is given in Appendix B. The subject of errors was oscillatory and does display certain wave features. discussed and an important reference was cited.

As previously stated in our introduction, It is important to note that even though exact examples of problems with time changing bound- solutions are sometimes possible for a rather large ary conditions are evident in the cylinders of class of problems, the exact solution is not always internal combustion engines, on industrial proc- in a form that readily yields numerical results. If esses where thermal cycling of a system occurs, numerical data is wanted for various times, the and in space applications where instrument amount of computer time needed to evaluate the packages are subjected to wide periodical varia- exact solution may well be much larger than the tions in temperature. Using the techniques that computation time needed to obtain a numerica) we have presented, students can inyesigate a wide solution by the difference technique that we have variety of practical, but perhaps analytically presented in this paper. An example of this is well difficult, problems.

demonstrated by the last problem of this paper.

The time required to sum the series of the exact **V. CONCLUSIONS**

solution to insure convergence to the third sig In this paper we have presented several ideas nificant digit was sixty times larger than that for that are central to the numerical solution of partial obtaining the same result by the difference equa differential equations. Our paper is intended for tion method.

**APPENDIX A**

In this appendix, we present the program that was used to obtain the data shown in Fig. 3. The program is written in FORTRAN IV and was executed on a Burroughs 5500.

**2*0***

**10 FILE 1 =TTY, UNIT=REMOTE**

**DI*M*ENSION *A*P(21), AB(21) 30 C THE ARRAYS AP AND AB SHALL REPRESENT THE VARIOUS TE*M*P DISTRIBUTIONS. 40 C THE *MAXIM*UM *T*IME OF INTEREST IS TIMAX 50 C THE TIME BETWEEN DATA OUTPUT IS DELT 60 C THE NATURAL TIME INCRE*M*ENT IS TNAT 70**

**TNAT=.151; TIMAX**=7*5*.5; DELT=15.1 **80 C Q AND N ARE LOOP COUNTERS**

**Q=0; N=0 100 C INITIALIZING THE DI*M*ENSIONED ARRAYS AP(I) TO ZERO AN**D AB(1) TO TO) **110**

**DO 11=1,21; AP(I)=0 120** 1 AB(I) = 100 **130**

**AB(1)=0; AB(2)=0**

**WRITE(1,20); WRITE(1,30); WRITE(1,20) 150**

**DO 2 K=1,21; KK=K-1 160 2 WRITE(1,40)KK, AB(K) 170 C INCRE*M*ENTING THE COUNTER Q BY ONE AND CALCULATING THE NEW TE*M*P 180 C DISTRIBUTION AT TIME (N\*DELT+Q\*TNAT) SEC. 190** 4 Q=Q+1 200

DO 51=2,20 **210 5 AP(I)=*1*2*./*3.)\*A**B(1)+(1./*6*.)\*(**AB(1-1)+-AB(1+1)) 220 C CHECKING TO SEE IF Q\*TNAT IS EQUAL TO DELT; IF SO SET** 230 C Q=**O AND WRITE OUT DATA, IF NOT, CONTINUE TO CALCULATE THE 240 C NEXT TEMPERATURE DISTRIBUTION. 2*5*0**

**IF(Q\*TNAT- DELT)6,8,8** 2606 Q=Q+1.

**140**

*JP Volume 41 / 528*

*R. A. Kobiske and J. L. Hock*

**270 280 290**

**300**

**310 320**

DO 71=2,20 7 AB(1)=(2./3.)\*AP(I)+11.*/*6.)\*(AP(1-1)+API+11)

fF(Q\*TNAT-DELT)4, 10, 10 8 Q=0; N=N+1; WRITE(1,20); XNN=N\*DELT; DO 3 K=1,21; KK=K-1 **3 WRIT**E(1,50)XNN,KK,AP(K); WRITE(1,20]; IF(N\***DELT -- TI*M*AX/6, 12, 12** 10 Q=0; N=N+1; WRITE(1,20); XNN=N\*DELT; DO 15 K=1,21; KK=K-1 **1*5* WRITE**(1,50)XNN,KK, AB(K); WRITE(1,20); IF(N\*DELT – TIMAX)4, 12, 12 **20 FORMAT**I*A)* **30 FOR*M*AT("THE ORIGINAL DATA I**S'') 40 FOR*M*AT("T(",12," CM) = ", IF8.3) **50 FOR*M****A*T*(*"TE*M*PI", 1F5.1," SEC,",12," CM) = ", 1F8.3) **12 STOP; END**

**330**

**3*40***

**350 360 *3*7*0* 380**

**APPENDIX B**

In Sec. III of this paper we made reference to an exact Fourier solution for the initial value problem:

*T(*0*,t) =T(L, t) =*0°C,

*T(*1,0)=*To*=100°C,

x=0, *L.*

This solution is readily found by using a standard Fourier analysis technique:

*T(*x, t) = ¿ *(4T./N*) exp[-(*Nra/L)24*] sin[N1 *(x/L)].*

**N=1,3,5**

In Sec. IV-B a copper sphere was subjected to the following initial condition:

*pra*,

*T(a*,0) =0°C, T(r, 0) =*T,*= 100°C,

rt*a*.

The exact solution for this problem is:

T+0,

*T(*r, t) = *2T*,(-1)N+1 exp[-(N*ra/a)24*] sin[*Nar/a*]/[(N*71/a*)],

***N*=1** *T(*0, t) = 3*T*(1*, t) - 3T (*2, *t)* +*T*(3*,t)*,

where the first equation was found by a Fourier series technique and the second by a three point interpolation scheme.

In Sec. IV-C, a spherical diffusion problem with time varying boundary conditions was solved numerically. The exact solution may be found with the aid of Laplace transforms. The solution that we obtained is given by:

21?*q?T*,

T(r, t) =

*T(r, t) =*

a

at, sin*(*Na*r/a)* {*(Noa/a*)2 sinut-w coswt twexp[- (N*ra/a)*24]} *(*-1) *N*-1N*2 –*

*(*N*or/a*)[*(Nra/a)*+w2]

***N=1***

N=1

*T(0, 1) =37(1, 1)-3T (2,1)*+*T(3, 1*) *T'(a, t) =T*o sinut

*524 / April 1978*

A*pril 1978*

17. W. Sears, *Mechanics*, W*ave Motion, and Heat* was never published by him. For the student who is (Addison-Wesley, Reading, Mass., 1959), p. 526.

interested in error analysis the reading of this paper is ? F. W. Sears, Ref. 1, pp. 524, 515.

highly recommended. 3 G. G. O'Brien, M. A. Hyman, and S. Kaplan, J. Math. 4 G. G. O'Brien, Ref. 3, p. 226. Phys. 29, 223 (1951). The stability error analysis that is 5G. G. O'Brien, Ref. 3, p. 227. presented in this reference was developed by J. Von Neu G. G. O'Brien, Ref. 3, p. 235. **ma**nn and was applied by him to a wide variety of differ ?H. W. Reddick and F. H. Miller, *Advanced Mathe* ence and differential equations during World War II, but *matics for Engineer*s (Wiley, New York, 1957), p. 403.

**Classical Limit of the Hydrogen Atom\***

LOWELL S. BROWN *Physics Department University of Washington Seattle, Washington 98195* (Received 20 November 1972; revised 15 December 1972)

A *wavepacket solution for the hydrogen atom in the region of large principal quantum number n is constructed. This wavepacket follows a classical circular orbit. It has a width on the order of n-1/2 times the size of the orbit.*

servation of energy and angular momentum forbid any transverse spreading of the wavepacket as time passes. On the other hand, there is no constraint to it spreading out along the orbit. Indeed, an optimally prepared packet will spread along a fraction of the orbit that is on the order of

number of revolutions*/n) 1/*2. For microscopic systems (such as the hydrogen atom itself) excited to macroscopic dimensions, *n*~104, and the width and spreading of the wavepacket are significant. But for truly macroscopic systems the principal quantum number is enormous (n-1020 to 1040), and the width and spreading are completely insignificant.

We begin our construction by recalling that a bound state of the hydrogen atom is described by the values of the total angular momentum *(1)* and its 2 component *(m*) in addition to the principal quantum number *(*n*)*. The wavefunction may be separated in spherical coordinates,

*Vi*mn(r) =*y-Hunt*(r) Ym(0*, 0).*

In general, the radial wavefunction obeys

{-*(da/dr*2)+*[(1*+1)/2]

+0(r) + Kni?}*U*ni(n) =0,

(2)

In many circumstances, the WKB approxima tion can be employed to construct a wavepacket solution to the Schrödinger equation that follows the classical trajectory and exhibits the classical limit of quantum mechanics. This solution, however, is not valid at turning points of the classical motion. Such a situation, and one of particular interest, occurs in the case of the simple circular orbit of a particle bound in a Coulomb potential. Here the particle is always at a turning point. It is the purpose of this note to construct a quantum wavepacket for systems of a hydrogen like character with a large principal quantum number n. This wavepacket follows the cor- responding classical circular? orbit to within a fractional width on the order of *n=1/*2. The con

with the bound state energy given by

*Eni= -(1*12 K*n*i?*/2m*) <0.

*(*3)

For the specific case of the Coulomb potential

V(r)=-*(2m/+2) (Ze-/r)*.

(4)

*AJP Volume 41 / 525*