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Numerical Solution to Transient Heat Flow Problems

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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 convergence 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.

I. INTRODUCTION

In our everyday experiences we are all familiar with the process of diffusion. A drop of black ink will diffuse when placed in a container of water; heat will diffuse toward your hand when you hold a metal bar in a flame. Other diffusion phenomena include neutron diffusion in the moderator around a reactor or neturon source, diffusion current is very important in a consideration of moving charge carriers in semi-conductor devices, and introduction of impurity atoms into solids by a diffusion process is important in the area of electronic devices. In many cases of practical interest, diffusion conduction processes occur under conditions where certain boundary conditions 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 significance 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.

II. THE DIFFUSION EQUATION AND A DIFFERENCE COUNTERPART

A. The One-Dimensional Diffusion Equation

The general form for the diffusion equation in a homogeneous medium is given as:[1]

$$\alpha^2\nabla^2 T = \partial T/\partial t \tag{1}$$

where T, for the problems considered in this paper, will represent temperature in degrees Celsius, t represents time in seconds, and α is the diffusivity with units of cm/sec$^{1/2}$. One can

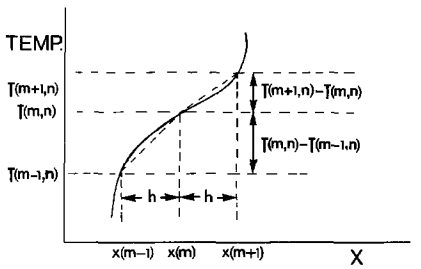

FIG. 1. A general curve of temperature vs linear distance for a particular time t.

show that α^2 is related to certain material parameters of the medium by:[2] $\alpha^2 = k/\rho c$, where k is the thermal conductivity, ρ is the material density, and c is the specific heat capacity.

In one dimension, ∇^2 has the form $\partial^2/\partial x^2$. Thus, in this representation, Eq. (1) becomes:

$$\alpha^2 \partial^2 T/\partial x^2 = \partial T/\partial t. \quad (2)$$

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,[1] and also in many other general physics texts. Since its inclusion here would add nothing new, we will omit this consideration.

B. The Difference Equation

Consider a solid of length L. We represent this distance by an integer number of equal subintervals 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 to $t = n\Delta t$, 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:

$$(\text{slope})_2 = [T(m+1, n) - T(m, n)]/h,$$
$$(\text{slope})_1 = [T(m, n) - T(m-1, n)]/h.$$

In a finite difference form, $\partial^2 T/\partial x^2$ can be approximated by the following expression:

$$\partial^2 T/\partial x^2 = \partial(\text{slope})/\partial x \cong [(\text{slope})_2 - (\text{slope})_1]/h.$$

This yields:

$$\partial^2 T/\partial x^2 \cong [T(m+1, n) + T(m-1, n) - 2T(m, n)]/h^2. \quad (3)$$

Similarly, a finite difference form of $\partial T/\partial t$ is:

$$\partial T/\partial t \cong [T(m, n+1) - T(m, n)]/\Delta t. \quad (4)$$

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

$$T(m, n+1) = T(m, n) + (\alpha^2 \Delta t/h^2) \times [T(m+1, n) + T(m-1, n) - 2T(m, n)]. \quad (5)$$

Solution to this equation gives the temperature at point $x(m)$ for some advanced time $t(n+1)$ in terms of what it was at point $x(m-1)$, $x(m)$, 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 $x=0$ and $x=L$, one can map the time evolution of the system from the difference Eq. (5).

C. Errors

It turns out that the above difference equation does not describe the actual physical situation for all values of $\beta = \Delta t \alpha^2/h^2$. What 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 considered only a small finite number of points. This greatly simplified picture 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 β, 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,[3] let D represent the exact solution of the partial differential Eq. (2), and Δ the exact solution of the

TABLE I. Convergence and stability are shown for $\alpha^2\Delta t/h^2=\frac{1}{4}$ in the difference equation

$$T(m, n+1)=T(m, n)+(\alpha^2\Delta t/h^2)[T(m+1, n)+T(m-1, n)-2T(m, n)].$$

$n\backslash m$	0	1	2	3	4
0	0	1	1	1	0
1	0	$\frac{3}{4}$	$1(\epsilon)$	$\frac{3}{4}$	0
2	0	$(5/8)(\frac{1}{4}\epsilon)$	$(7/8)(\frac{1}{2}\epsilon)$	$(5/8)(\frac{1}{4}\epsilon)$	0
3	0	$(17/32)(\frac{1}{4}\epsilon)$	$(3/4)(3\epsilon/8)$	$(17/32)(\frac{1}{4}\epsilon)$	0
4	0	$(29/64)(7\epsilon/32)$	$(41/64)(5\epsilon/16)$	$(29/64)(7\epsilon/32)$	0
5	0	$(99/256)(12\epsilon/64)$	$(140/256)(17\epsilon/64)$	$(99/256)(12\epsilon/64)$	0

partial finite difference Eq. (5). Let N represent the numerical solution of the partial difference equation. $(D-\Delta)$ is called the truncation error; it arises because of the finite distance between points of the difference mesh. To find the conditions under which $\Delta\rightarrow D$ is the problem of convergence. $(\Delta-N)$ is called the numerical error; in our discussion it is limited to round off error. To find the conditions under which $(\Delta-N)$ remains small as time advances is the problem of stability. In order to illustrate the dependence of convergence/stability upon the parameter $\beta=\alpha^2\Delta t/h^2$, we will introduce the following example:

Let $T(x,\ 0)=1$ for $0<x<1$, $T(0,\ t)=0$, $T(1, t)=0$, with $\beta=\frac{1}{4}, \frac{3}{4}$, and $h=\frac{1}{4}$. In the matrix tables that are displayed in Table I and Table II, we show the numerical solutions to this problem for the two values of the β parameter. For the moment, ignore the numbers in the brackets. In Table I it is not difficult to believe that, even though the values obtained for any given h are not smooth, the numbers obtained by this process would approach the exact solution of the partial differential equation as h and Δt were decreased. In Table II the solution is in a state of oscillation; it would be very difficult to believe that this solution could represent the exact solution. We would say that the solution of Table I is convergent while that of Table II is divergent. In order to study the stability let us introduce a numerical error ϵ at $T(2, 1)$ and follow this error as it propagates. In Table I the error decays, while in Table II, the error oscillates in sign and grows as time is advanced. We would say that the solution

TABLE II. The breakdown of both convergence and stability is shown for $\alpha^2\Delta t/h^2=\frac{3}{4}$ in the difference equation

$$T(m, n+1)=T(m, n)+(\alpha^2\Delta t/h^2)[T(m+1, n)+T(m-1, n)-2T(m, n)].$$

$n\backslash m$	0	1	2	3	4
0	0	1	1	1	0
1	0	$\frac{1}{4}$	$1(\epsilon)$	$(\frac{1}{4})$	0
2	0	$(5/8)(3\epsilon/4)$	$-(1/8)(-\frac{1}{2}\epsilon)$	$(5/8)(3\epsilon/4)$	0
3	0	$-(13/32)(-3\epsilon/4)$	$1(11\epsilon/8)$	$-(13/32)(-3\epsilon/4)$	0
4	0	$(61/64)(45\epsilon/32)$	$-(71/64)(-29\epsilon/16)$	$(61/64)(45\epsilon/32)$	0
5	0	$-(335/256)(-132\epsilon/64)$	$(294/128)(193\epsilon/64)$	$-(335/256)(-132\epsilon/64)$	0

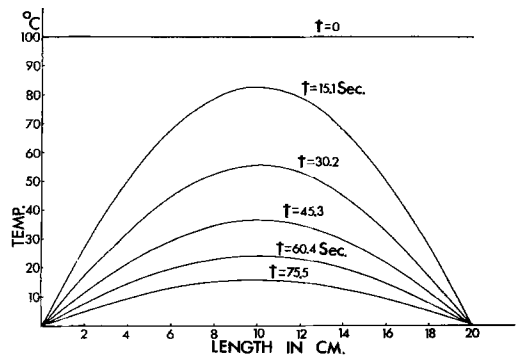

FIG. 2. Temperature distributions in a rectangular copper bar.

of Table I is stable while that of Table II is unstable. One can show that[4] the error ϵ obeys the same difference equation as the temperature distribution $\Delta(m, n)$. This is important in that it indicates that ϵ and the transient part of $\Delta(m, n)$ usually have the same growth properties. The word "usually" was used rather than "invarably," because one must consider the effect of an initial condition which influences $\Delta(m, n)$ but not the error ϵ.

It can be shown[5] that a stable solution results for $\beta \leq \frac{1}{2}$. Thus, $\beta = \frac{1}{2}$ separates the region of stability, where errors decay, from the region of instability, where errors grow. In order to establish some criterion for convergence, we again reference O'Brien.[6] Consider the same problem that we employed to distinguished between convergence and stability, O'Brien has given an exact solution to our difference Eq. (5) for this problem:

$$T(x, t) = \frac{2}{M} \sum_{j=1,3,5}^{M-1} \cot\left(\frac{j\pi}{2M}\right) \times \sin(\Pi j x) \left[1 - 4\beta \sin^2\left(\frac{\Pi j}{2M}\right)\right]^k$$

where: $x = j/M$, $t = k\Delta t$, $\beta = \alpha^2 \Delta t/h^2$, and M represents the number of cell spacings.

As time increases, k increases, and for the last factor to remain finite, β must be less than or equal to $\frac{1}{2}$.

Thus, the choice of:

$$\beta = \alpha^2 \Delta t/h^2 \leq \tfrac{1}{2} \qquad (6)$$

insures both stability and convergence of the difference equation.

III. A ONE DIMENSIONAL HEAT FLOW PROBLEM

Consider a rectangular piece of copper of length L, with insulated sides, ends held at 0°C, and an initial temperature distribution given by:

$$T(m, 0) = 100°\text{C}, \quad m \neq 0, \quad L/h;$$
$$T(0, n) = T(L/h, n) = 0°\text{C}.$$

The difference Eq. (5) was programmed (See Appendix A) for this problem and the numerical results are displayed in Fig. 2. In order to have an integer number of spatial divisions between zero and L, it is convenient to choose h and allow the stability relationship shown in Eq. (6) to determine Δt.

The previously defined constant, α^2, has the value of 1.10407 cm²/sec, for copper.[2] The value of L was chosen to be 20 cm, $\beta = \frac{1}{6}$, and $h = 1$ cm. This produces a time step of $\Delta t = 0.150956$ sec.

In Appendix B an exact Fourier series solution to the above problem is given. This series is summed to insure a convergence to six significant digits for the times displayed in Fig. 2. The results of a numerical comparison of the above methods indicate a maximum deviation of 0.36%. The result of this comparison also indicates that the above numerical technique is stable and convergent. This gives one confidence that the application of this technique to more difficult, 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 consider the ends held at different temperatures. The final steady state temperature distribution is already familiar to students who have had a first course in Physics and is simply a linear distribution between the end point temperatures.

A more interesting situation arises if we consider two materials with equal thermal conductivities k, but with different densities ρ and heat

capacities, c_p. From general physics, one knows that the steady state heat current depends only upon the thermal conductivity; however, for the transient response, as the steady state is approached, the transient heat current also depends upon both the material density and heat capacity. Thus, the above materials will have identical steady state heat currents for equal boundary conditions at the ends, but will have much different transient responses in the decay toward the steady state. Students might expect, from consideration of steady state heat flow, that the termal conductivity alone will control the results rather than the density and heat capacity in addition to the conductivity. Physically, the amount of heat stored per unit volume depends on the product of heat capacity and density; in a time changing situation, this storage consideration is important while, in steady state heat transfer all elments of mass have fixed amounts of energy. The heat current depends only upon the ability of the medium to transfer heat by the conductivity mechanism. Each element of mass acts as a source or a sink for the energy being transferred, while the energy associated with each element is held constant. In a consideration of transient flow, the condition of constant energy per mass cell does not hold. In order to investigate this effect, a student might look up the material parameters of nickel steel (70% Ni) and also those of lead. The above problem could be programmed, and the resulting transient temperature distributions compared. After a little search, he will find that several other pairs of materials are also suitable to display the above effect.

IV. A THREE-DIMENSIONAL HEAT FLOW PROBLEM WITH SPHERICAL SYMMETRY

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[7]:

$$\alpha^2[\partial^2 T/\partial r^2+(2/r)(\partial T/\partial r)]=\partial T/\partial t, \quad (7)$$

where r represents a radial distance. Consider the transformation:

$$T(r, t)=V(r, t)/r.$$

It is easy to show that if $T(r, t)$ is a solution to Eq. (7), $V(r, t)$ is a solution to Eq. (2) with x replaced by r:

$$\alpha^2\partial^2 V(r, t)/\partial r^2=\partial V(r, t)/\partial t. \quad (8)$$

A difference counterpart for Eq. (8) has already been developed in Sec. II–B, Eq. (5), and is restated here using the transformed variable $V(m, n)$:

$$V(m, n+1)=V(m, n)+(\alpha^2\Delta t/h^2)\times[V(m+1, n)+V(m-1, n)-2V(m, n)].$$

Under the conditions of stability and convergence [Eq. (6)] we have:

$$V(m, n+1)=\tfrac{2}{3}V(m, n)+\tfrac{1}{6}[V(m+1, n)+V(m-1, n)], \quad (9)$$

where a value of $\frac{1}{6}$ has been choosen for the parameter $\alpha^2\Delta t/h^2$. One advantage to using the above transformation is that the previously discussed error analysis can now be applied directly to this new three-dimensional problem. Thus, we can form a numerical solution to this new differential equation by applying previously developed techniques. Using the theory developed above we shall discuss the programming of a practical problem.

B. A Three-Dimensional Heat Flow Problem

Consider the situation where a copper sphere of radius a is initially held at a constant temperature T_0. The surface of the sphere is then brought into contact with an ice bath of temperature 0°C. We wish to plot the spatial temperature distribution for different values of time.

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

$$T(a, t)=0°\text{C}, \quad \text{surface at } 0° \text{ } \forall \text{ time}$$

$$T(r, 0)=T_0=100°\text{C}, \quad r\neq a. \quad \text{start at } 100° \text{ uniform}$$

The problem now proceeds as in Sec. III. The

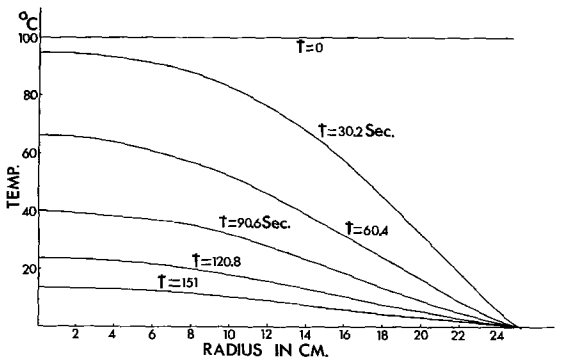

FIG. 3. Temperature distributions in a copper sphere.

don't divide by r=0

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. $T(0, t)$ is found by making use of a three point interpolation scheme. An exact solution to this problem is displayed in Appendix B. The results of a numerical comparison of the difference technique with the exact solution are identical to those of the previous problem.

C. A Spherical Diffusion Problem With 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 surface temperature according to:

$$T(a, t) = T_0 \sin\omega t.$$

Following the previous discussion, we again wish to program the 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 transformation $V(r, t) = rT(r, t)$ has been applied. Recall, $T(m, n)$ corresponds to the temperature distribution in the spherical space, and $V(m, n)$ is the associated temperature distribution in the equivalent linear medium. Under this transformation the new boundary and initial conditions become:

$$V(a, t) = aT_0 \sin\omega t,$$
$$V(0, t) = V(r, 0) = 0.$$

The condition $V(0, t) = 0$ must be imposed to insure that $T(0, t)$ will be finite at $r = 0$. As in the previous 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 difference scheme, this series was summed to 2000 terms and compared with the results of the numerical difference technique. For this comparison, the time was advanced to 200 sec. The results agreed to within 3%.

One can observe a steady build-up in temperature at the center 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 variable technique, with a real separation constant, one cannot introduce the time changing boundary condition. One must introduce a complex separation constant and proceed from there. The equation 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

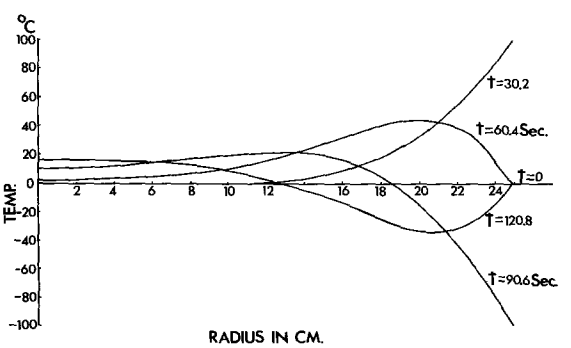

FIG. 4. Temperature distributions in a copper sphere which is subject to sinusoidal surface temperature variations.

technique. The oscillatory behavior of this system is interesting from the standpoint that one does not usually associate a diffusion process with a wave type of motion. While the situation that we have discussed is not strictly wave motion, it is oscillatory and does display certain wave features.

As previously stated in our introduction, examples of problems with time changing boundary conditions are evident in the cylinders of internal combustion engines, on industrial processes where thermal cycling of a system occurs, and in space applications where instrument packages are subjected to wide periodical variations in temperature. Using the techniques that we have presented, students can invesigate a wide variety of practical, but perhaps analytically difficult, problems.

V. CONCLUSIONS

In this paper we have presented several ideas that are central to the numerical solution of partial differential equations. Our paper is intended for the undergraduate physics and engineering student. Three problems of increasing difficulty were presented, and computer solutions were graphically displayed. Exact series solutions were given in Appendix B. The subject of errors was discussed and an important reference was cited.

It is important to note that even though exact solutions are sometimes possible for a rather large class of problems, the exact solution is not always in a form that readily yields numerical results. If numerical data is wanted for various times, the amount of computer time needed to evaluate the exact solution may well be much larger than the computation time needed to obtain a numerical solution by the difference technique that we have presented in this paper. An example of this is well demonstrated by the last problem of this paper. The time required to sum the series of the exact solution to insure convergence to the third significant digit was sixty times larger than that for obtaining the same result by the difference equation 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.

```
 10  FILE 1=TTY, UNIT=REMOTE
 20        DIMENSION AP(21),AB(21)
 30  C  THE ARRAYS AP AND AB SHALL REPRESENT THE VARIOUS TEMP DISTRIBUTIONS.
 40  C  THE MAXIMUM TIME OF INTEREST IS TIMAX
 50  C  THE TIME BETWEEN DATA OUTPUT IS DELT
 60  C  THE NATURAL TIME INCREMENT IS TNAT
 70        TNAT=.151; TIMAX=75.5; DELT=15.1
 80  C  Q AND N ARE LOOP COUNTERS
 90        Q=0; N=0
100  C  INITIALIZING THE DIMENSIONED ARRAYS AP(I) TO ZERO AND AB(I) TO T(0)
110        DO 1 I=1,21; AP(I)=0
120      1 AB(I)=100
130        AB(1)=0; AB(2)=0
140        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  INCREMENTING THE COUNTER Q BY ONE AND CALCULATING THE NEW TEMP
180  C  DISTRIBUTION AT TIME (N*DELT+Q*TNAT) SEC.
190      4 Q=Q+1
200        DO 5 I=2,20
210      5 AP(I)=(2./3.)*AB(I)+(1./6.)*(AB(I-1)+AB(I+1))
220  C  CHECKING TO SEE IF Q*TNAT IS EQUAL TO DELT; IF SO SET
230  C  Q=0 AND WRITE OUT DATA, IF NOT, CONTINUE TO CALCULATE THE
240  C  NEXT TEMPERATURE DISTRIBUTION.
250        IF(Q*TNAT-DELT)6,8,8
260      6 Q=Q+1
```

```
270        DO 7 I=2,20
280      7 AB(I)=(2./3.)*AP(I)+(1./6.)*(AP(I-1)+AP(I+1))
290        IF(Q*TNAT-DELT)4, 10, 10
300      8 Q=0; N=N+1; WRITE(1,20); XNN=N*DELT; DO 3 K=1,21; KK=K-1
310      3 WRITE(1,50)XNN,KK,AP(K); WRITE(1,20); IF(N*DELT-TIMAX)6, 12, 12
320     10 Q=0; N=N+1; WRITE(1,20); XNN=N*DELT; DO 15 K=1,21; KK=K-1
330     15 WRITE(1,50)XNN,KK,AB(K); WRITE(1,20); IF(N*DELT-TIMAX)4, 12, 12
340     20 FORMAT(//)
350     30 FORMAT("THE ORIGINAL DATA IS")
360     40 FORMAT("T(",I2," CM) = ", 1F8.3)
370     50 FORMAT("TEMP(", 1F5.1," SEC,",I2," CM) = ", 1F8.3)
380     12 STOP; END
```

APPENDIX B

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

$$T(0, t) = T(L, t) = 0°\text{C},$$

$$T(x, 0) = T_0 = 100°\text{C}, \qquad x \neq 0, L.$$

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

$$T(x, t) = \sum_{N=1,3,5}^{\infty} (4T_0/N\pi) \exp[-(N\pi\alpha/L)^2 t] \sin[N\pi(x/L)].$$

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

$$T(a, 0) = 0°\text{C}, \qquad r = a,$$

$$T(r, 0) = T_0 = 100°\text{C}, \qquad r \neq a.$$

The exact solution for this problem is:

$$T(r, t) = \sum_{N=1}^{\infty} 2T_0(-1)^{N+1} \exp[-(N\pi\alpha/a)^2 t] \sin[N\pi r/a]/[(N\pi r/a)], \qquad r \neq 0,$$

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

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:

$$T(r, t) = \frac{2\pi^2\alpha^2 T_0}{a^2} \sum_{N=1}^{\infty} (-1)^{N-1} N^2 \frac{\sin(N\pi r/a)\{(N\pi\alpha/a)^2 \sin\omega t - \omega\cos\omega t + \omega\exp[-(N\pi\alpha/a)^2 t]\}}{(N\pi r/a)[(N\pi\alpha/a)^4 + \omega^2]}$$

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

$$T(a, t) = T_0 \sin\omega t$$

[1] F. W. Sears, *Mechanics, Wave Motion, and Heat* (Addison–Wesley, Reading, Mass., 1959), p. 526.

[2] F. W. Sears, Ref. 1, pp. 524, 515.

[3] G. G. O'Brien, M. A. Hyman, and S. Kaplan, J. Math. Phys. **29**, 223 (1951). The stability error analysis that is presented in this reference was developed by J. Von Neumann and was applied by him to a wide variety of difference and differential equations during World War II, but was never published by him. For the student who is interested in error analysis the reading of this paper is highly recommended.

[4] G. G. O'Brien, Ref. 3, p. 226.

[5] G. G. O'Brien, Ref. 3, p. 227.

[6] G. G. O'Brien, Ref. 3, p. 235.

[7] H. W. Reddick and F. H. Miller, *Advanced Mathematics for Engineers* (Wiley, New York, 1957), p. 403.

Classical Limit of the Hydrogen Atom*

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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.

In many circumstances, the WKB approximation 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.[1] 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 corresponding classical circular[2] orbit to within a fractional width on the order of $n^{-1/2}$. The conservation 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, $n\sim10^4$, and the width and spreading of the wavepacket are significant. But for truly macroscopic systems the principal quantum number is enormous ($n\sim10^{20}$ to 10^{40}), 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 (l) and its z component (m) in addition to the principal quantum number (n). The wavefunction may be separated in spherical coordinates,

$$\psi_{lmn}(\mathbf{r}) = r^{-1}u_{nl}(r)\,Y_l^m(\theta,\phi). \tag{1}$$

In general, the radial wavefunction obeys

$$\{-(d^2/dr^2)+[l(l+1)/r^2] + \mathcal{U}(r)+\kappa_{nl}^2\}u_{nl}(r)=0, \tag{2}$$

with the bound state energy given by

$$E_{nl}=-(\hbar^2\kappa_{nl}^2/2m)<0. \tag{3}$$

For the specific case of the Coulomb potential

$$\mathcal{U}(r)=-(2m/\hbar^2)(Ze^2/r). \tag{4}$$