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The two-dimensional hydrogen atom with a logarithmic potential energy function

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Recently, a "shooting" method has been used to obtain exact expressions for eigenvalues and eigensolutions of the two-dimensional hydrogen atom. This paper shows that the shooting method is easy for undergraduate students to understand and implement numerically. The highly accurate approximations for both eigenvalues and eigensolutions are then used to contrast the two-dimensional and three-dimensional hydrogen atoms. Finally, previous methods for solving the two-dimensional hydrogen atom are compared with the shooting method.

I. INTRODUCTION

Understanding the physical world is inextricably linked with a clear understanding of the quantum mechanical model that has proved so successful in describing atomic processes. Recently, applications of this model to physical systems in other spatial dimensions[1] have been made in the hope of both illuminating the special characteristics of the three-dimensional world and obtaining rare "exact" solutions to the quantum theory. One such attempt has been the study of the hydrogen atom in two-dimensional space. This is the atom formed by the attraction of two electrically charged particles, an electron of two-dimensional charge $-q$ and a proton of two-dimensional charge q. It is common knowledge[2–4] that the correct mutual electrostatic potential energy function, the one satisfying Gauss' theorem, for such a system in two-dimensional space is a logarithmic function of the distance r separating the two particles. Neglecting relativistic and magnetic effects, this means that the time-independent Schrödinger equation in polar coordinates for the relative motion of this system is

$$[-\hbar^2\nabla^2/(2\mu)+q^2\ln(r/r_0)]\psi(r,\phi)=E\psi(r,\phi), \quad (1)$$

where $\mu=m_pm_e/(m_p+m_e)$ is the reduced two-dimensional mass of the proton–electron system, $\hbar$ is the two-dimensional Planck constant divided by 2π, and r_0 is a scale constant. The goal is to find the energy eigenvalues E and the corresponding (nontrivial) eigensolutions ψ of Eq. (1) which are bounded and square integrable in two-dimensional space:

$$\int_0^{2\pi}\int_0^{\infty}|\psi(r,\phi)|^2 r\,dr\,d\phi<\infty. \quad (2)$$

The chief difficulty in achieving this goal is the logarithmic potential energy term that causes a branch point singularity at $r=0$ in Eq. (1). This renders ineffective the power series techniques that lead to exact solutions for such cases as the Coulomb potential cr^{-1} and the harmonic oscillator potential cr^2. Previous work on the system (1)–(2) has been in one of two directions: Approximate the eigenvalues using variational techniques[5,6] or represent the solutions to (1) in terms of infinite series of functions.[7,8] Recently, one of the authors[9] has developed the theoretical framework for a new technique that simultaneously yields the eigenvalues and eigensolutions of the system (1)–(2). The purpose of this paper is to show that this new unified method is both easy to comprehend and computationally effective. To this end, four undergraduate engineering students, coauthors Eveker, Jost, Nelson, and Stroh, implemented this method numerically on a Micro-VAX II computer; the results obtained are highly accurate approximations of the eigenvalues and corresponding eigensolutions.

It is the belief of the authors that the method will prove general in nature and be applicable for solving the Schrödinger equation with a wide variety of potential energy functions including the Coulomb and harmonic oscillator potentials. Certainly students in a quantum mechanics course would find the highly geometric nature of the method more natural and intuitive than the classical power series technique. Furthermore, certain aspects of the quantum theory (e.g., the principal or total quantum number) would arise naturally from geometric properties of the eigensolutions (e.g., the number of their real zeros).

II. THE METHOD OF SOLUTION

The analysis of the system (1)–(2) begins with some mathematical reductions. The radial symmetry of the potential energy function permits separation of the variables in Eq. (1). This, together with the requirement that $\psi(r,\phi+2\pi)=\psi(r,\phi)$, yields

$$\psi(r,\phi)=R(r)\exp(il\phi)/\sqrt{2\pi}, \tag{3}$$

where l is any integer; the radial part $R=R(r)$ satisfies

$$K_l(R)=ER, \tag{4}$$

where

$$K_l=\frac{d^2}{dr^2}+r^{-1}\frac{d}{dr}-l^2r^{-2}-\left(\frac{2\mu}{\hbar^2}\right)q^2\ln\left(\frac{r}{r_0}\right).$$

The square integrability condition reduces to

$$\int_0^\infty |R(r)|^2 r\,dr<\infty. \tag{5}$$

The transformation from the independent variable r in Eq. (4) to the variable u defined by

$$\ln\left(\frac{r}{r_0}\right)=\left(\frac{u}{2}\right)+\left(\frac{E}{q^2}\right) \tag{6}$$

simplifies the radial eigenvalue Eq. (4). The results are the equivalent equation

$$\frac{d^2R}{du^2}-\left[\left(\frac{l^2}{4}\right)+\sigma u\exp(u)\right]R=0, \tag{7}$$

where $\sigma=\mu q^2 r_0^2\exp(2E/q^2)/(4\hbar^2)$ and the equivalent square integrability condition

$$\int_{-\infty}^\infty |R(u)|^2\exp(u)\,du<\infty. \tag{8}$$

Thus solving the eigenvalue problem (1)–(2) reduces to solving the eigenvalue problem (7)–(8). The calculations of this work are based on the results in Ref. 9 concerning the solution of the latter problem; consequently, the basic underlying ideas will be outlined at this point.

Fix a positive integer l and let σ be any positive real number.[10] Let $R=S_\sigma(u)$ denote the solution to Eq. (7), which satisfies the initial conditions $R(0)=1$, $R'(0)=l/2$. It is easy to show that $S_\sigma(u)$ is bounded below by $\exp(lu/2)$ on the positive u axis so the definite integral

$$c(\sigma)=\int_0^\infty [S_\sigma(w)]^{-2}\,dw \tag{9}$$

is finite. If $R=T_\sigma(u)$ is the solution to Eq. (7), which satisfies the conditions

$$R(0)=1,\quad R'(0)=(l/2)-[c(\sigma)]^{-1}, \tag{10}$$

then it is not hard to prove that as u approaches infinity, $T_\sigma(u)$ approaches zero so rapidly that "half" of condition (8) is satisfied:

$$\int_0^\infty |T_\sigma(u)|^2\exp(u)du<\infty.$$

From this it is clear that if $T_\sigma(u)$ is bounded as u approaches negative infinity, then this σ value will be an eigenvalue of (7)–(8) and $R=T_\sigma(u)$ will be an eigensolution. A careful analysis shows that as the parameter σ increases, the number of real zeros of T_σ either increases or remains the same. The eigenvalues and eigensolutions occur at those σ values where the number of real zeros of T_σ jumps abruptly by one. The reason for this is that as σ increases, the additional real zero of T_σ first appears at negative infinity. At such a σ value, $T_\sigma(u)$ is then bounded as u approaches negative infinity.

For example, when σ is sufficiently close to zero, $T_\sigma(u)$ is always positive and diverges to infinity as u approaches negative infinity. Moreover, if σ is increased just beyond a certain critical value, call it σ_1, then $T_\sigma(u)$ always possesses a real zero and diverges to negative infinity as u approaches negative infinity (see Fig. 1). This critical value is equal to the supremum or least upper bound of the σ values

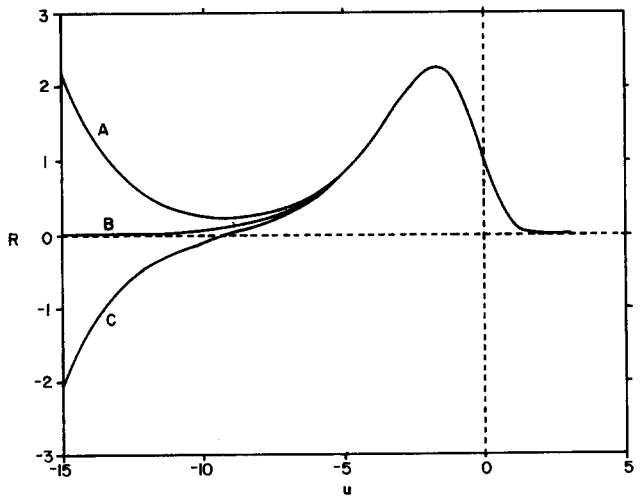

Fig. 1. T_σ curves for σ values near the critical value σ_1 when $l=1$. A: $R=T_\sigma(u)$, where $\sigma<\sigma_1$; B: $R=T_{\sigma_1}(u)$; C: $R=T_\sigma(u)$, where $\sigma>\sigma_1$.

for which T_σ has no real zeros; in symbols,

$$\sigma_1 = \sigma_1(l) = \sup\{\sigma > 0 : T_\sigma \text{ has no real zeros}\}.$$

It can be shown that $T_{\sigma_1}(u)$ approaches zero as u approaches negative infinity so σ_1 is an eigenvalue of (7)–(8) and T_{σ_1} is an eigensolution. In general, if l remains fixed and σ_n is defined by

$$\sigma_n = \sigma_n(l) = \sup\{\sigma > 0 : T_\sigma \text{ has exactly } n-1 \text{ real zeros}\}, \quad (11)$$

then it can be shown that $T_{\sigma_n}(u)$ approaches zero as u approaches negative infinity. In this way, infinite sequences of eigenvalues $\sigma_1(l) < \sigma_2(l) < \sigma_3(l) < \cdots$ and corresponding eigensolutions $T_{\sigma_1}, T_{\sigma_2}, T_{\sigma_3}, \ldots$ of (7)–(8) are constructed. This procedure, using Eq. (11) to generate eigenvalue–eigensolution pairs for the system (7)–(8), will be referred to as the shooting method in analogy with a technique for solving two-point boundary value problems.[11]

We conclude this section by formally stating several properties of the function T_σ which will be needed when the numerical computations of eigenvalues and eigensolutions are described in Sec. III.

(1) For each $\sigma > 0$, T_σ has no zeros in the positive u axis.

(2) If the equation $(l^2/4) + \sigma u \exp(u) = 0$ has a real solution, let u_1 denote the smallest such solution; otherwise, set $u_1 = +\infty$. Then T_σ has at most one zero in the interval $-\infty < u < u_1$.

(3) If u_0 is a zero of T_σ then $T_\sigma(u)$ changes its algebraic sign at $u = u_0$.

(4) If σ is not an eigenvalue of (7)–(8), then $|T_\sigma(u)|$ tends to infinity as a constant multiple of $\exp(-lu/2)$ as u approaches negative infinity.

(5) The number of real zeros of T_σ is a nondecreasing function of σ.

(6) For each positive integer n, T_{σ_n} has exactly $n-1$ real zeros.

(7) T_σ has at least n real zeros whenever $\sigma > \sigma_n$.

The proofs of these and other statements in this section, as well as further properties of the eigenvalues $\sigma_n(l)$ and the eigensolutions T_{σ_n}, can be found in Ref. 9.

III. NUMERICAL IMPLEMENTATION OF THE METHOD

The eigenvalues $\sigma = \sigma_n(l)$ of (7)–(8) are given by Eq. (11). In order to turn this theoretical formulation into a computationally effective procedure, one must be able to determine accurately and efficiently the number of real zeros of T_σ for each $\sigma > 0$. The approach taken in this work was to use a highly accurate numerical method[12] to solve the initial value problem (7)–(10), for which $R = T_\sigma(u)$ is the solution. It was assumed that the number of real zeros of T_σ was equal to the number of sign changes in the numerical solution. Neglecting errors due to imprecise machine arithmetic, this assumption is valid provided the stepsize is sufficiently small and σ is not an eigenvalue [see properties (3) and (4) of Sec. II].

By properties (1) and (2) of Sec. II, all the real zeros of T_σ are in the negative u axis and all, save possibly one, are in a predetermined finite interval. Furthermore, when σ is not an eigenvalue and $l \neq 0$, $|T_\sigma(u)|$ diverges exponentially as u approaches negative infinity [see property (4) of Sec. II], making it easy to tell when to quit searching for more real zeros of T_σ. These additional facts allow the numerical solution of (7)–(10) to be carried out on a finite interval of the negative u axis. In this work, for example, the interval $-50 \leqslant u \leqslant 0$ was more than sufficient to determine the eigenvalues $\sigma_n(l)$ to eight significant digits for the parameter ranges $0 \leqslant l \leqslant 4$ and $1 \leqslant n \leqslant 5$.

One straightforward approach to solving the initial value problem numerically (7)–(10) consists of the following three steps:

(i) Solve Eq. (7) numerically on a sufficiently large finite interval of the positive u axis subject to the initial conditions $R(0) = 1$, $R'(0) = l/2$ to obtain approximate values for $R = S_\sigma(u)$.

(ii) Approximate the value of $c(\sigma)$ given by Eq. (9) using a numerical quadrature method together with the approximate values of $S_\sigma(u)$ from step (i).

(iii) Use the approximate value for $c(\sigma)$ from step (ii) and solve Eq. (7) numerically on a sufficiently large finite interval of the negative u axis subject to the initial conditions $R(0) = 1$, $R'(0) = (l/2) - [c(\sigma)]^{-1}$ to get approximate values for $R = T_\sigma(u)$.

The chief difficulty with this procedure proved to be that the numerical quadrature in step (ii) produced relatively inaccurate approximations for $c(\sigma)$. This effectively doomed the entire approach since the numerical solution in step (iii) was quite sensitive to even small changes in $c(\sigma)$. To give some feeling for the accuracy requirements, it became apparent in subsequent computations that between 12 and 14 significant digit accuracy in $c(\sigma)$ was needed to achieve 8 significant digit accuracy in the eigenvalues $\sigma_n(l)$.

Consequently, a different procedure was devised in which steps (i) and (ii) were replaced by a more accurate method for determining $c(\sigma)$. This new procedure was based on finding the solution $R = R_c(u)$ to Eq. (7) on the positive u axis subject to the initial conditions

$$R(0) = 1, \quad R'(0) = (l/2) - c^{-1}, \quad (12)$$

where c is a positive parameter. It is easily seen that $cR_c(u) = [c - c(\sigma)]S_\sigma(u) + c(\sigma)T_\sigma(u)$ and since $S_\sigma(u)$ increases to infinity and $T_\sigma(u)$ decreases to 0 as u approaches infinity, it follows that $c_1 < c(\sigma) < c_2$ if and only if $R_{c_1}(u)$ and $R_{c_2}(u)$ approach negative and positive infinity, respectively, as u approaches infinity. This led to the following method for numerically solving the initial value problem (7)–(10).

(i′) Find a bracket $[c_L, c_R]$ for $c(\sigma)$ by twice numerically solving the initial value problem (7)–(12) on a sufficiently large interval of the positive u axis to obtain solutions $R_{c_L}(u)$ and $R_{c_R}(u)$ which diverge to negative and positive infinity, respectively, as u approaches infinity. Due to the rapid growth in $S_\sigma(u)$ with increasing u, the interval $0 \leqslant u \leqslant 10$ proved sufficiently large in all cases.

(ii′) Let $c_M = (c_L + c_R)/2$ denote the midpoint of the previous bracket for c_σ and numerically solve Eq. (7) on a sufficiently large interval of the positive u axis subject to the initial conditions (12) with $c = c_M$. If $R_{c_M}(u)$ diverges to negative infinity with increasing u, set $c_L = c_M$; otherwise, if $R_{c_M}(u)$ diverges to infinity set $c_R = c_M$. The result is a new bracket $[c_L, c_R]$ for $c(\sigma)$ which is half the length of the previous bracket.

(iii′) Repeat the bisection procedure of step (ii′) until a

Table I. Tight upper bounds for the eigenvalues σ of the system (7)–(8) for the parameter ranges $0 \leqslant l \leqslant 4$ and $1 \leqslant n \leqslant 5$.

	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$
$n=1$	0.358 286 07	1.999 5675	4.999 3233	9.358 1924	15.076 210
$n=2$	3.466 2085	6.955 3283	11.849 450	18.115 901	25.747 087
$n=3$	9.727 1731	15.017 795	21.772 834	29.924 231	39.452 551
$n=4$	19.133 753	26.203 520	34.795 887	44.812 685	56.222 450
$n=5$	31.684 119	40.519 049	50.931 655	62.797 960	76.075 308

sufficiently accurate approximation for $c(\sigma)$ is obtained. In the present work, 16 significant digit accuracy in $c(\sigma)$ was sufficient.

(iv′) Use the approximate value for $c(\sigma)$ from step (iii′) and solve Eq. (7) numerically on a sufficiently large finite interval of the negative u axis subject to the initial conditions $R(0)=1$, $R'(0)=(l/2)-[c(\sigma)]^{-1}$. (As previously mentioned, the interval $-50 \leqslant u \leqslant 0$ sufficed.)

The method outlined in steps (i′) through (iv′) proved to be reliable in determining the number of real zeros of T_σ for each $\sigma > 0$. This permitted the numerical determination of the eigenvalues of (7)–(8) using the following technique. Fix $\sigma_L > 0$ and suppose that T_{σ_L} has m real zeros. Properties (5) and (6) of Sec. II imply that $\sigma_L \leqslant \sigma_{m+1}$. If the value of σ is increased beyond σ_L then eventually a value σ_R is reached for which T_{σ_R} has $m+1$ real zeros; but then $\sigma_{m+1} < \sigma_R$ by properties (5) and (6). In this way a bracket $[\sigma_L, \sigma_R]$ is obtained for σ_{m+1}. This $(m+1)$th eigenvalue can be approximated, at least in principle, to any desired accuracy by repeatedly bisecting the bracket. If σ denotes the midpoint of $[\sigma_L, \sigma_R]$, then set $\sigma_L = \sigma$ if T_σ has m real zeros; otherwise, set $\sigma_R = \sigma$ if T_σ has $m+1$ real zeros. In this manner a new bracket for σ_{m+1} is obtained that is half the length of the previous bracket. Note that this iterated bisection procedure for computing the $(m+1)$th eigenvalue simultaneously yields successively better approximations of the eigensolution $T_{\sigma_{m+1}}$ since numerical values for the convergents, T_{σ_L} and T_{σ_R}, are generated in the course of determining the number of their real zeros.

The shooting method was implemented on a Micro VAX II computer using FORTRAN 77 programs and double precision arithmetic; copies of the source programs are available from the authors upon request. The decision to implement the method by shooting Eq. (7) rather than (4) stemmed from a desire to maximize numerical efficiency. The first derivative of the dependent variable is absent in (7); consequently, it could be efficiently solved using an extension of Runge–Kutta methods to second-order differential equations first introduced by Nyström.[13] The classical fifth-order Nyström method[14] was used to obtain preliminary values for $\sigma_n(l)$. Refined values of $c(\sigma)$, $T_\sigma(u)$, and $\sigma_n(l)$ were then determined using a highly accurate tenth-order Nyström method developed by Hairer.[12] An approximate one-third reduction in CPU time resulted from using this method to solve Eq. (7) as opposed to employing a Runge–Kutta method of equivalent accuracy to solve (4).[12] This significant improvement in numerical efficiency had a pedagogical cost, however. The logarithmic transformation (6) increased the complexity of the mathematical analysis and replaced the physically meaningful variable r with the artificial variable u. Admittedly, the undergraduate students would more easily have understood shooting the original equation (4). In retrospect, the substitution $X(r) = r^{1/2}R(r)$ in (4) might have been closer to optimal because it results in the numerically efficient equation

$$X'' + \{(2\mu/\hbar^2)[E - q^2 \ln(r/r_0)] + (\tfrac{1}{2} - l)(\tfrac{1}{2} + l)r^{-2}\}X = 0,$$

which still retains many pedagogically attractive features.

IV. THE EIGENVALUES AND EIGENSOLUTIONS

The theoretical results and their numerical implementation yielded the estimates given in Table I for the eigenvalues σ of the system (7)–(8) when the parameters l and n were in the ranges $0 \leqslant l \leqslant 4$ and $1 \leqslant n \leqslant 5$. The entry corre-

Table II. σ eigenvalues for the system (7)–(8) converted from γ eigenvalues of (13) using the relation $8\sigma = \exp(2\gamma)$. These were determined by Asturias and Aragón[6] and Reiser.[5]

	$l=0$		$l=1$		$l=2$		$l=3$		$l=4$
	Ref. 6	Ref. 5	Ref. 6	Ref. 5	Ref. 6	Ref. 5	Ref. 6	Ref. 5	Ref. 6
$n=1$	0.358 38 $\pm 2\times10^{-5}$	0.53501 $\pm 3\times10^{-3}$	1.999 66 $\pm 8\times10^{-5}$	1.9995 $\pm 1\times10^{-4}$	4.9996 $\pm 4\times10^{-4}$	4.9993 $\pm 2\times10^{-4}$	9.358 25 $\pm 2\times10^{-4}$	9.358 63 $\pm 8\times10^{-4}$	15.0769 $\pm 1\times10^{-3}$
$n=2$	3.446 82 $\pm 1\times10^{-4}$	3.959 82 $\pm 4\times10^{-3}$	6.955 82 $\pm 3\times10^{-4}$	6.95874 $\pm 1\times10^{-4}$	11.8634 $\pm 7\times10^{-4}$	11.8532 $\pm 1\times10^{-3}$	18.1161 $\pm 4\times10^{-4}$	18.1197 $\pm 1\times10^{-2}$	
$n=3$	9.728 29 $\pm 2\times10^{-4}$	10.5804 $\pm 6\times10^{-3}$	15.0187 $\pm 3\times10^{-4}$	15.0684 $\pm 6\times10^{-3}$	21.7797 $\pm 1\times10^{-2}$	21.8172 $\pm 2\times10^{-2}$			
$n=4$	19.1369 $\pm 4\times10^{-4}$	20.5220 $\times 8\times10^{-4}$	26.2052 $\pm 5\times10^{-3}$	26.5279 $\pm 2\times10^{-3}$					
$n=5$	32.219 $\pm 7\times10^{-2}$	34.10 $\pm 1\times10^{-1}$							

sponding to a given pair of integers l and n in Table I is a tight upper bound for σ in the sense that if 1 is subtracted from the last digit of the entry then a lower bound for σ results.

Asturias and Aragón[6] based their eigenvalue computations on the differential equation

$$\left\{\frac{1}{z}\left[\frac{d}{dz}\left(z\frac{d}{dz}\right)\right]-\frac{l^2}{z^2}-\ln(z)+\gamma\right\}R(z)=0, \qquad (13)$$

which is equivalent to Eq. (4) [and hence to Eq. (7)] via the substitution $z=\beta^{1/2}r$ where $\beta=2\mu q^2/\hbar^2$ and $\gamma=E/q^2$. The estimates for the eigenvalues γ obtained by Reiser[5] and by Asturias and Aragón[6] were reported in Table I of Ref. 6. These were converted to σ values using the relationship $8\sigma=\exp(2\gamma)$ and are displayed in Table II of this work. The obvious discrepancies between the approximations for the case $l=0$ in Table II are discussed in Asturias and Aragón[6] and a convincing argument is given for the greater accuracy of those of Ref. 6. It is apparent that the approximations for the eigenvalues displayed in Table I are in general agreement with those in Table II; when $l=0$ the approximations of Table I are in close agreement with those of Ref. 6 in Table II. Observe that almost without fail the eigenvalue approximations in Table I are less than the corresponding entries in Table II. This is consistent with the claim of greater accuracy for the approximations in Table I because the variational techniques used in Refs. 5 and 6 produce upper bounds for the eigenvalues.[15] Figure 3 displays in graphical form the values obtained by the authors for the first three eigensolutions to (7)–(8) when $l=1$.

When $l=0$ in the eigenvalue problem (7)–(8), theoretical difficulties arise because the differential operator $d^2/du^2-\sigma u\exp(u)$ is not self-adjoint on its natural domain, the space of all twice differentiable functions $f(u)$ satisfying the square integrability condition (8) and for which $R(u)=[d^2/du^2-\sigma u\exp(u)]f(u)$ also satisfies (8). A startling consequence of this nonself-adjointness is that when $l=0$ there exist square integrable solutions of the form (3) to Eq. (1) for every real number E,[9] a situation that is untenable on physical grounds. Although a rigorous mathematical resolution of the self-adjointness of $d^2/du^2-\sigma u\exp(\mu)$ is still lacking, it appears likely to the

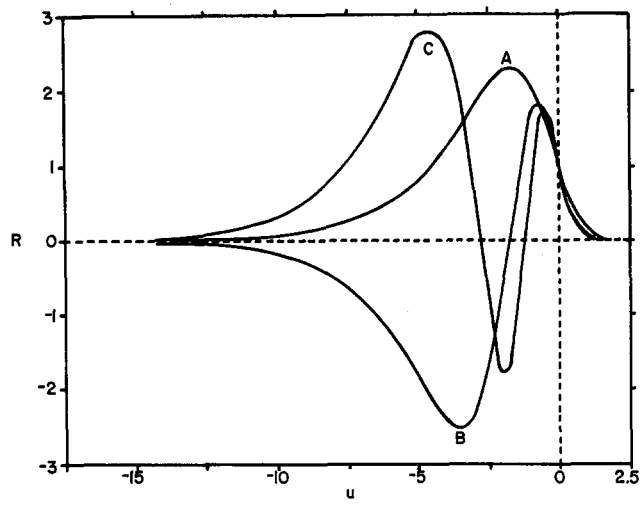

Fig. 3. The first three eigensolutions to the system (7)–(8) when $l=1$, normalized so $R(0)=1$. A: $R=T_{\sigma_1}(u)$; B: $R=T_{\sigma_2}(u)$; C: $R=T_{\sigma_3}(u)$.

authors that the problem can be resolved by insisting that the solutions to (7) be bounded as well as satisfy inequality (8). It was assumed in this paper that when $l=0$ the eigenvalues σ_n $(n=1,2,3,\ldots)$ of the system (7)–(8) could be obtained from Eq. (11) and that the corresponding eigensolutions $T_{\sigma_n}(u)$ approached a nonzero constant value as u approached negative infinity (see Fig. 2). In light of the uncertain theoretical foundation for the shooting method computations of this paper when $l=0$, it was reassuring to the authors to obtain close agreement with the $l=0$ eigenvalues computed in Ref. 6 using an altogether different method (see column 1 in Tables I and II).

The primary physical interest, however, is not in solutions to the transformed system (7)–(8), but rather in those for the radial system (4)–(5). As discussed in Sec. II, solutions for the two systems are in one-to-one correspondence. Specifically, suppose E and σ are related by the equation $\sigma=\mu q^2 r_0^2\exp(2E/q^2)/(4\hbar^2)$ and define the function $u_\sigma(r)=2\ln(r/r_0)-\ln[4\hbar^2/(\mu q^2 r_0^2)]$. Then $R=T_\sigma[u_\sigma(r)]$ is a solution to (4)–(5) whenever R

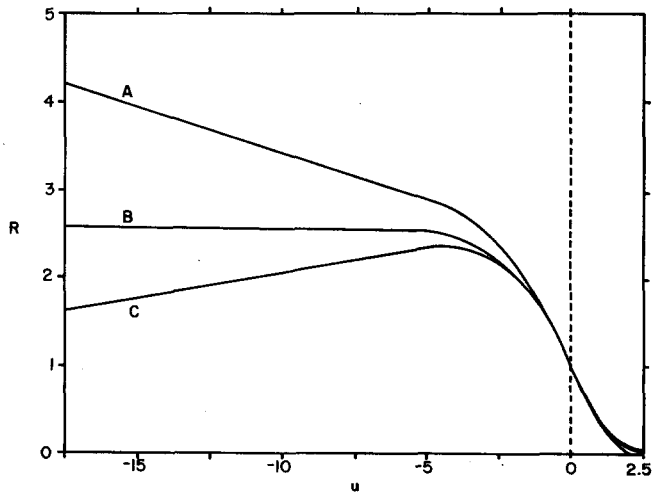

Fig. 2. T_{σ_n} curves for σ values near the critical value σ_1 when $l=0$. A: $R=T_{\sigma_1}(u)$, where $\sigma<\sigma_1$; B: $R=T_{\sigma_1}(u)$; C: $R=T_{\sigma_1}(u)$, where $\sigma>\sigma_1$.

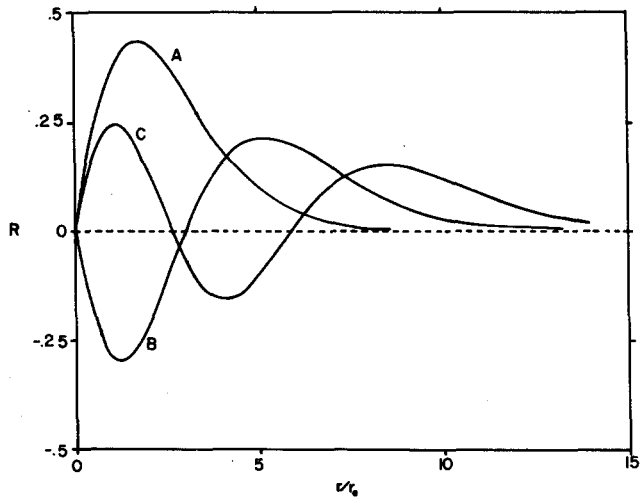

Fig. 4. The first three eigensolutions to the system (4)–(5) when $l=1$, normalized so $\int_0^\infty |R(r)|^2 r\,dr=1$. A: $R=c_1T_{\sigma_1}[u_{\sigma_1}(r)]$; B: $R=c_2T_{\sigma_2}[u_{\sigma_2}(r)]$; C: $R=c_3T_{\sigma_3}[u_{\sigma_3}(r)]$.

$= T_\sigma(u)$ is a solution to (7)–(8). Figure 4 presents graphs obtained in this manner for the first three eigensolutions to (4)–(5) in the case $l = 1$.

In connection with electron interferences in the electric field generated by a cylindrical capacitor in three-dimensional space, Gesztesy and Pittner[7] have studied an equation that is nearly identical with (7):

$$\left(\frac{d^2}{dx^2} - l^2\right) y(x) = \lambda x \exp(2x) y(x). \tag{14}$$

Reference 7 shows that the solution to (14), which behaves appropriately at negative infinity, $y(x)\exp(-lx) \to 1$ as $x \to -\infty$, can be expressed as an infinite series of exponential polynomials:

$$y_l(\lambda,x) = \exp(lx) \sum_{n=0}^{\infty} [\lambda \exp(2x)]^n p_{n,l}(x). \tag{15}$$

Here, $p_{n,l}(x)$ is a polynomial of degree n defined recursively by putting $p_{0,l}(x) = 1$ and

$$\left(4n(n+l) + 2(2n+l)\frac{d}{dx} + \frac{d^2}{dx^2}\right) p_{n,l}(x)$$

$$= x p_{n-1,l}(x), \quad \text{for } n = 1,2,3,\ldots .$$

The eigensolutions of the system (7)–(8) can be related to the solutions of (14) which are given by Eq. (15). To accomplish this, fix a nonnegative integer l and define

$$Y(\lambda,x) = [y_l(\lambda,0)]^{-1} y_l(\lambda,x). \tag{16}$$

If $\sigma_n = \sigma_n(l)$ is the nth eigenvalue of (7)–(8), then it is easy to show that the nth eigensolution is given by

$$T_{\sigma_n}(u) = Y(8\sigma_n, u/2). \tag{17}$$

The procedure based on using Eqs. (15)–(17) to obtain the eigensolutions to the system (7)–(8) will be referred to as the infinite series method.

Table III compares numerical values for $T_{\sigma_1}(u)$ yielded by the shooting and infinite series methods when $l = 1$. In the latter method, 1.999 5674 was used as the value of σ_1. A step size of 0.01 was employed in the tenth-order numerical differential equation solver portion of the shooting method to calculate the approximations for $T_{\sigma_1}(u)$ displayed in column 2. The values for $Y(8\sigma_1, u/2)$ in column 3 were computed by truncating the infinite series (15) so the index of summation extended from $n = 0$ to $n = 15$. It is apparent that values derived using the two methods agree quite closely. For example, their relative difference $2|T_{\sigma_1}(u) - Y(8\sigma_1, u/2)|/[|T_{\sigma_1}(u)| + |Y(8\sigma_1, u/2)|]$, is less than one-half percent over the interval $-16 \leqslant u \leqslant 2$. This corresponds to an error of less than five parts of 1000 over the range of physical distances $0.001\,342 \leqslant r/r_0 \leqslant 10.87$ if, following Ref. 6, the scale constant is chosen to be $r_0 = \hbar/(q\sqrt{2\mu})$.

When u is negative, the values for the eigensolutions in column 3 of Table III are almost certainly more reliable than those in column 2. There are two reasons for this. First, the infinite series in (15) is uniformly convergent on the negative x axis.[7] Second, the calculated values of $Y(8\sigma_1, u/2)$ did not change appreciably when the index of the partial sum approximating (15) ranged from $n = 0$ to $n = 25$. The shooting method approximation in column 2, on the other hand, is unstable and will eventually diverge if carried out far enough on the negative u axis [see property (4) on Sec. II]. For positive values of u, however, the situation is reversed; the shooting method values in column 2 are more reliable than those in column 3 resulting from the infinite series method. This is due to the slow convergence of the infinite series (15) on the positive x axis. For instance, when $\lambda = 8\sigma_1(1) \approx 16$, $x = 1$, and $n = 15$ the exponential factor multiplying $p_{n,l}(x)$ in (15) is approximately 10^{31}.

The accuracy of the shooting method approximations depends ultimately on the accuracy of the numerical differential equation solver. It seemed appropriate, therefore, to test the accuracy of the tenth-order Nyström[12] method employed in this work by numerically solving several initial value problems whose analytical solutions were known. In each case a step size of 0.01 was used. The first test case was the relatively nonstiff differential equation $(1+u^2)^2 R'' - 8u^2 R = 6u$ with the constraints $R(0) = 0$ and $R'(0) = -1$. The analytical solution $R = -u(1+u^2)^{-1}$ behaves somewhat like the first eigensolution $T_{\sigma_1}(u)$ near the origin on the negative u axis. The first ten significant digits of the numerical solution agreed with the analytical solution throughout $-50 \leqslant u \leqslant 50$. The second case was the mildly stiff differential equation $R'' - R = 0$ subject to the initial conditions $R(0) = R'(0) = 1$. The analytical solution $R = \exp(u)$ behaves asymptotically on the negative u axis like the eigensolutions to (7)–(8) when $l = 2$. Over

Table III. Comparison of numerical values obtained for the first eigensolution to the system (7)–(8) when $l = 1$ using two techniques: the shooting method (column 2) and the infinite series method (column 3).

u	$R = T_{\sigma_1}(u)$	$R = Y(8\sigma_1, u/2)$	Relative difference (%)
2.0	$2.315\,400\,256\,2218 \times 10^{-3}$	$2.293\,545\,926\,424 \times 10^{-3}$	0.363 201 743
0.0	1.000 000 000 000	1.000 000 000 000	0.000 000 000
−2.0	2.248 328 960 316	2.248 329 064 162	0.000 004 619
−4.0	1.249 601 222 744	1.249 601 314 153	0.000 007 315
−6.0	$4.998\,537\,335\,558 \times 10^{-1}$	$4.998\,538\,145\,130 \times 10^{-1}$	0.000 016 196
−8.0	$1.867\,497\,400\,279 \times 10^{-1}$	$1.867\,498\,852\,677 \times 10^{-1}$	0.000 077 772
−10.0	$6.888\,446\,967\,144 \times 10^{-2}$	$6.888\,483\,322\,302 \times 10^{-2}$	0.000 527 769
−12.0	$2.535\,146\,855\,572 \times 10^{-2}$	$2.535\,244\,377\,708 \times 10^{-2}$	0.003 846 730
−14.0	$9.324\,650\,668\,778 \times 10^{-3}$	$9.327\,296\,148\,333 \times 10^{-3}$	0.028 366 793
−16.0	$3.424\,169\,082\,496 \times 10^{-3}$	$3.431\,357\,954\,600 \times 10^{-3}$	0.209 724 857
−18.0	$1.242\,787\,737\,622 \times 10^{-3}$	$1.262\,328\,157\,433 \times 10^{-3}$	1.560 041 193
−20.0	$4.112\,687\,292\,092 \times 10^{-4}$	$4.643\,846\,944\,421 \times 10^{-4}$	12.131 732 530

the interval $-10 \leqslant u \leqslant 0$, the global error of the numerical solution was just 8.8×10^{-13}. However, the numerical solution subsequently deteriorated and by $u = -19$, only the first significant digit was correct. The third case involved the extremely stiff differential equation $R'' + (1-u^2)R = 0$. The analytical solution that satisfies the initial conditions $R(0) = 1$, $R'(0) = 0$ is $R = \exp(-u^2/2)$, a function whose asymptotic behavior on the positive u axis resembles that of an eigensolution to (7)–(8). The global error of the numerical solution was only 1.7×10^{-14} over the interval $0 \leqslant u \leqslant 4$. However, just two significant digits of the numerical solution were correct at $u = 6$, and by $u = 10$ it had begun to diverge to infinity. It is the considered opinion of the authors that the accuracy of the numerical approximations for the eigensolutions to (7)–(8) is roughly similar to case 1 near the origin and analogous to cases 2 and 3 asymptotically on the negative and positive u axes, respectively.

V. ANALYSIS AND CONCLUSIONS

The accurate determinations of eigenvalues and eigensolutions presented in Sec. IV confirm and extend the understanding of the two-dimensional hydrogen atom. In particular, the ordering of electron energy levels in the two-dimensional hydrogen atom, reported previously in Refs. 5 and 6, was verified:

$$\begin{aligned}\sigma_1(0) &< \sigma_1(1) < \sigma_2(0) < \sigma_1(2) < \sigma_2(1) < \sigma_1(3) \\ &< \sigma_3(0) < \sigma_2(2) < \sigma_3(1) \\ &< \sigma_1(4) < \sigma_2(3) < \sigma_4(0) < \cdots,\end{aligned}$$

or equivalently:

$$1s < 1p < 2s < 1d < 2p < 1f < 3s < 2d < 3p < 1g < 2f < 4s < \ldots,$$

where 1,2,3,4,... denote the values of the radial quantum number n and $s,p,d,f,g,\ldots$ denote the values $l = 0,1,2,3,4,\ldots$, respectively, for the angular quantum number.

The highly accurate eigenvalue approximations also encourage speculation concerning the functional dependence of the eigenvalue σ on the radial and angular quantum numbers, n and l. Table IV illustrates a simple empirical relationship

$$\sigma_n(l) \approx f(n,l) = (3n+l)(n+l-1)/2, \tag{18}$$

which gives general agreement with the eigenvalues in Table I. Realize, however, that the values in Table IV are crude approximations.

The functional relationship in (18) has some theoretical justification. In Ref. 9 it is proven that if l is nonzero, there exist numbers $k_1 = k_1(l)$ and $k_2 = k_2(l)$ such that

$$k_1 [n/\ln(n)]^2 \leqslant \sigma_n(l) \leqslant k_2 n^2 \tag{19}$$

Table IV. Approximate eigenvalues obtained from the empirical formula (18).

	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$
$n=1$	0	2	5	9	14
$n=2$	3	7	12	18	25
$n=3$	9	15	22	30	39
$n=4$	18	26	35	45	56
$n=5$	30	40	51	63	76

whenever n is sufficiently large. Thus, if l is a fixed positive integer, $f(n,l)$ has the same general asymptotic behavior as $\sigma_n(l)$ when n tends to infinity.

Asymptotic expressions for the energy eigenvalues of the two-dimensional hydrogen atom also follow from (19). Recall from Sec. II that σ is related to the energy E in the Schrödinger equation (1) by $\sigma = \mu q^2 r_0^2 \exp(2E/q^2)/(4\hbar^2)$. Solving for E in terms of σ yields the expression

$$E(n,l) = (q^2/2)\ln[4\hbar^2\sigma_n(l)/(\mu q^2 r_0^2)] \tag{20}$$

for the energy eigenvalue corresponding to the radial and angular quantum numbers, n and l. Appealing to (19) gives numbers $c_1 = c_1(l)$ and $c_2 = c_2(l)$ such that

$$c_1 \ln[n/\ln(n)] \leqslant E(n,l) \leqslant c_2 \ln(n)$$

whenever n is sufficiently large and l is nonzero. In particular, it is not difficult to show that $E(n,l)$ is asymptotic to $q^2 \ln(n)$ when n tends to infinity and l is a fixed positive integer.

This asymptotic behavior of $E(n,l)$ points out one fundamental difference between the two-dimensional and three-dimensional hydrogen atoms: The electron energy levels for the two-dimensional hydrogen atom are unbounded[5] while those for the three-dimensional hydrogen atom are of bounded energy. Specifically, the energy eigenvalues of the three-dimensional hydrogen atom are given by

$$\mathscr{E}(N) = -\mu q^4/(2\hbar^2 N^2), \tag{21}$$

where $N = 1,2,3,\ldots$ denotes the total quantum number.[16] That is, $N = n_r + l + 1$ where $n_r = 0,1,2,\ldots$ is the radial quantum number and $l = 0,1,2,\ldots$ is the orbital–angular-momentum quantum number. Consequently, the only possible electron energy levels in the three-dimensional hydrogen atom lies between $-\mu q^4/(2\hbar^2)$ and zero. Implications of the unboundedness of electron energy levels in the two-dimensional hydrogen atom have been addressed in Ref. 5 for such physical processes as ionization and electrical conduction in two-dimensional matter.

Equations (20) and (21) and Table I reveal another basic difference between the two-dimensional and three-dimensional hydrogen atoms: the degeneracy of the electron energy levels. The dependence of $\mathscr{E}(N)$ on the sum of n_r and l in Eq. (21) makes clear the degeneracy of the energy eigenvalues in the three-dimensional hydrogen atom, at least when n_r and l are nonzero; to each such energy eigenvalue there corresponds N^2 linearly independent eigensolutions.[17] On the other hand, Table I and Eq. (20) make clear that the energy eigenvalues $E(n,l)$ in the two-dimensional hydrogen atom are distinct, at least when the radial and angular quantum numbers are in the ranges $1 \leqslant n \leqslant 5$ and $0 \leqslant l \leqslant 4$. It has been shown that this distinctness extends to all energy eigenvalues $E(n,l)$ where $n \geqslant 1$ and $l \geqslant 0$.[4] The invariance of Eq. (4) under a change in the sign of l shows that $E(n,l) = E(n,-l)$. Consequently, when l is nonzero, Eq. (3) implies that there are two linearly independent eigensolutions to the Schrödinger equation (1) corresponding to each energy eigenvalue $E(n,l)$. When the angular quantum number is nonzero, the doubly degenerate nature of the electron energy levels in the two-dimensional hydrogen atom has been discussed in terms of the Bohr model.[5]

The accurate eigensolution determinations presented in Sec. IV clarify details in the understanding of the two-dimensional hydrogen atom. This work gives tangible illus-

trations of previous theoretical results concerning properties of the radial part[7,9] and makes it clear that the radial parts of the wave functions for the two-dimensional and three-dimensional hydrogen atoms are very similar. To be precise, recall that

$$R(\rho) = e^{-\rho/2}\rho^{l}L_{N+l}^{2l+1}(\rho) \tag{22}$$

is the radial part of the eigensolution ψ corresponding to the total and orbital-angular-momentum quantum numbers, N and l, in the Schrödinger equation for the three-dimensional hydrogen atom.[18] In Eq. (22), ρ is a nondimensionalized distance from the center of mass and $L_{N+l}^{2l+1}(\rho)$ denotes the associated Laguerre polynomial of degree $n_r = N - l - 1$. It follows from (22) that $R(\rho)$ possesses the three properties listed below:

(1) $R(\rho)$ has n_r real zeros in the interval $0 < \rho < +\infty$.

(2) $R(\rho)/\rho^{l}$ approaches a nonzero constant value as ρ approaches zero.

(3) $R(\rho)$ decays exponentially to zero as ρ tends to infinity.

References 7 and 9 show that the radial part of the wave function ψ of the two-dimensional hydrogen atom has these same properties provided $n_r = n - 1$, where $n = 1,2,3,...$ is the radial quantum number used in this investigation, and with the understanding that $R(\rho)/\rho^{|l|}$ replaces the expression in property (2), since $l = 0, \pm 1, \pm 2,...$ in the two-dimensional hydrogen atom. Figure 4 illustrates properties (1), (2), and (3) in an explicit manner for the radial part of the wave function for the two-dimensional hydrogen atom.

In contrast with variational methods[5,6] which are better suited for approximating eigenvalues than eigensolutions[19] and infinite series techniques[7,8] which yield solutions to the radial differential equation without identifying eigenvalues, the shooting method unifies the eigenvalue–eigensolution computations for the two-dimensional hydrogen atom. For this reason, the method possesses a distinct theoretical attractiveness. A major goal of this paper has been to demonstrate that, in addition to its theoretical appeal, the shooting method is effective as well from a computational standpoint. The eight significant digit eigenvalue approximations of Table I and the eigensolution values displayed in Table III, accurate to the millionths place over the range $-10 \leqslant u \leqslant 0$, effectively support this objective.

The sheer accuracy of the results, however, does not fully demonstrate the intrinsic advantages of the shooting method. First, a major advantage is that it produces both upper and lower bounds for each eigenvalue since a bracket $\sigma_L \leqslant \sigma_n \leqslant \sigma_R$ is maintained at each stage of the iterative approximation of the nth eigenvalue. This contrasts favorably with variational techniques that give only an upper bound for each eigenvalue.[15]

Second, the shooting method is a one-parameter method. For each fixed value of l, one varies the single parameter σ to pinpoint eigenvalues and eigensolutions of the system (7)–(8). Variational techniques, on the other hand, approximate the first n eigenvalues for the radial differential operator K_l in (4) using the eigenvalues of an associated $n \times n$ Hermitian matrix that is "close" to K_l, at least when n is large.[20] Thus a variational technique is a multiparameter method with the elements of the $n \times n$ matrix serving as parameters.

Regardless of whether or not the shooting method is computationally more efficient in determining eigenvalues than a variation technique, the fact that it is a one-parameter method contributes to a second goal of this paper: to show that the shooting method is easy to comprehend. Indeed, one can actually view the convergence process as the eigenvalue–eigensolution computations advance. Varying the parameter σ changes the slope with which the eigensolution candidate $R = T_\sigma(u)$ passes through the point (0,1) in the $u - R$ plane [see Eqs. (9) and (10)] and influences the general concavity of $R = T_\sigma(u)$ [see Eq. (7)]. An eigenvalue–eigensolution pair results when the parameter σ is fine tuned so as to make T_σ asymptotic to the negative u axis (see Fig. 1).[21] By contrast, for a variational method it is harder to grasp and hold in focus the more abstract, diffuse role of the coefficients of the $n \times n$ matrix in approximating the eigenvalues of K_l, especially when n is large.

Thus fewer parameters make the shooting method easier to visualize and comprehend than a variational technique. This, however, is not the sole reason why it is more intelligible. A careful examination of the theory upon which any variational technique is based leads to sophisticated mathematical concepts: infinite-dimensional Hilbert space, linear operators on Hilbert space, the representation of an operator with respect to an orthonormal basis for the space, and finite-dimensional projections of Hilbert space operators. The shooting method, in contrast, is based on elementary mathematical concepts. To grasp its theoretical foundations, one need not look beyond the radial differential equation; solution "waves" are sought that are bounded near the origin and approach zero as r tends toward infinity. Consequently, the conceptual simplicity of the shooting method enhances its understandability in comparison with a variational technique.

As previously discussed, a major advantage of the shooting method over the infinite series method is that the former unifies the eigenvalue–eigensolution computations. In the three-dimensional hydrogen atom, infinite series representations for solutions to the radial differential equation lead quickly to polynomial solutions and thus to eigenvalues, at least when the exponential decay at infinity has been suitably factored out [see Eq. (22)]. The analysis is not as simple in the case of the two-dimensional hydrogen atom and infinite series representations for the solutions have not yielded eigenvalues.

However, assuming the eigenvalues are somehow known, the infinite series method has certain distinct advantages over the shooting method in determining eigensolutions. First Eqs. (15)–(17) are more easily implemented on a computer and require substantially less CPU time to execute than the shooting method. Second, Eq. (15) shows very clearly the dependence of the eigensolution of the parameters l and λ, a definite aid in comprehending the infinite series method. Despite these advantages, however, recall from Sec. IV that the series in Eq. (15) converges very slowly on the positive x axis. Therefore, the infinite series method is not as computationally superior to the shooting method as it first appears. Incidentally, the slow convergence on the positive x axis dims any hope of implementing the shooting method using the function $y_l(\lambda,x)$ in Eq. (15) instead of $T_\sigma(u)$ as the eigensolution candidate.

Perhaps the most important advantage of the shooting method in comparison with the infinite series method is its promise in treating quantum mechanical systems with a spherically symmetric potential $V(r)$. In such situations the problem reduces to solving the radial equation

$$\frac{d^2R}{dr^2}+\left(\frac{n-1}{r}\right)\frac{dR}{dr}$$
$$+\left(\frac{2m}{\hbar^2}[E-V(r)]+\frac{k(l)}{r^2}\right)R=0 \tag{23}$$

subject to the condition[22]

$$\int_0^\infty |R(r)|^2 r^{n-1}\,dr<\infty. \tag{24}$$

Here, n is the spatial dimensionality of the physical system and $k(l)$ denotes the lth eigenvalue of the Laplace–Beltrami operator corresponding to the sphere in n-dimensional space.

If $p(r)=r^{n-1}$ and $q(r)=r^{n-1}\{(2m/\hbar^2)[E-V(r)]+k(l)/r^2\}$, Eq. (23) can be placed in the form

$$\frac{d}{dr}\left(p(r)\frac{dR}{dr}\right)+q(r)R=0. \tag{25}$$

A general result[23] concerning equations of the form (25) guarantees the existence of a "small" solution $R_0(r)$, one which has the property

$$R_0(r)/R_1(r)\to 0 \text{ as } r\to+\infty \tag{26}$$

for any solution $R_1(r)$ of (25) that is linearly independent of $R_0(r)$. A solution $R_0(r)$ that enjoys property (26) is called a principal solution of (25) at infinity and any solution $R_1(r)$ that is linearly independent of $R_0(r)$ is called a nonprincipal solution of (25) at infinity.

A principal solution of (23) at infinity is fundamental in solving the radial problem (23)–(24), for its asymptotic behavior gives the best chance of satisfying (24) among the solutions of (23). Reference 23 gives explicit representations for principal and nonprincipal solutions; in particular, a principal solution can always be constructed from any nonprincipal one via the formula

$$R_0(r)=R_1(r)\int_r^\infty \frac{[R_1(s)]^{-2}\,ds}{p(s)}. \tag{27}$$

The eigensolution candidate $T_\sigma(u)$ for the system (7)–(8) was produced in this manner.[9] The initial conditions in (10), which were used to define T_σ in Sec. II, were derived from a representation of the form (27). Conditions in (10) were used in this investigation to characterize T_σ rather than (27) because a numerical differential equation solver proved to be computationally more effective in approximating $T_\sigma(u)$.

Equipped with a principal solution $R_E(r)$ of (23) at infinity as the eigensolution candidate, the shooting method can be employed to solve the radial system (23)–(24). This consists of holding l fixed and adjusting the parameter E in Eq. (23) until $R_E(r)$ is bounded near zero. For any such value of E, the corresponding $R_E(r)$ should satisfy the condition in (24) thus making E and $R_E(r)$ an eigenvalue–eigensolution pair of the radial system. In this work, before applying the shooting method to the two-dimensional hydrogen atom, the radial system (4)–(5) on the interval $0<r<\infty$ was transformed into (7)–(8) on the interval $-\infty<u<\infty$ for reasons discussed earlier. Otherwise, the shooting method was applied exactly as described above. In particular, the parameter σ was adjusted so that $T_\sigma(u)$, a principal solution to (7) at positive infinity, was bounded near negative infinity. This resulted in a sequence of eigenvalue–eigensolution pairs σ and $T_\sigma(u)$ to (7)–(8).

We conclude with a list of problems and questions that arose in the course of this work and warrant further investigation.

(1) Find general conditions on the potential energy function $V(r)$ in the radial equation (23) which will ensure that the shooting method applied to (23)–(24) yields rigorous mathematical eigenvalue–eigensolution pairs E and $R_E(r)$.

(2) Employ the shooting method in other quantum mechanical systems which have a spherically symmetric potential energy function and obtain highly accurate numerical approximations for radial eigenvalue–eigensolution pairs.

(3) Compare the numerical efficiencies of the three methods for solving the radial eigenvalue problem of the two-dimensional hydrogen atom: the shooting method, variational techniques, and the infinite series method.

(4) Explore the mathematical subtleties inherent in the transformed radial system (7)–(8) of the two-dimensional hydrogen atom in the case when $l=0$. Specifically, is it possible to justify the assumption listed in Sec. IV that formed the basis for the $l=0$ calculations of this paper?

(5) Discuss and contrast the differences in the units for charge, mass, energy, and distance as exhibited in the two-dimensional and three-dimensional hydrogen atoms.

(6) Obtain exact mathematical expressions for the eigenvalues for the radial system (4)–(5) [or equivalently (7)–(8)] of the two-dimensional hydrogen atom. In particular, can the approximate empirical relationship in Eq. (18) for the eigenvalues $\sigma_n(l)$ be modified to give precise agreement with the computed values in Table I?

(7) Determine exact closed-form expressions in terms of elementary functions for the eigensolutions for the radial system of the two-dimensional hydrogen atom. To date, the only exact solutions to the transformed radial differential equation (14) are the decidedly open-form representations as infinite series of exponential polynomials [see Eq. (15)].[7]

(8) Extend the shooting method to solve the relativistic Dirac equation for the two-dimensional hydrogen atom with a logarithmic potential energy function.[24]

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[18]Reference 16, pp. 90–94.

[19]Reference 15, pp. 5, 9.

[20]Reference 15, p. 27.

[21]In this discussion it has been assumed that l is positive. If l is zero, σ should be adjusted so that $T_{,,}(u)$ approaches a nonzero constant value as u tends to negative infinity (see Fig. 2).

[22]M. Reed and B. Simon, *Methods of Modern Mathematical Physics* (Academic, New York, 1975), Vol. 2, pp. 160–161.

[23]P. Hartman, *Ordinary Differential Equations* (Wiley, New York, 1964), pp. 355–356.

[24]F. Gesztesy and L. Pittner, "Electrons in logarithmic potentials II. Solution of the Dirac equation," J. Phys. A **11**, 687–695 (1978).

Newton's first two laws of motion are not definitions

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Newton's first two laws of motion are often taken to be a definition of force. It is argued that they are true laws in that they make statements about the nature of the physical world. In particular, the first law can be viewed as asserting the existence of an ensemble of trajectories in a four-dimensional space along which force-free bodies, if they exist, would move. Such an ensemble, together with Newton's absolute time, constitute the essential ingredients of the underlying geometrical structure of Newtonian space-time. If this view is accepted, it is a relatively simple matter to describe how special and general relativity differ from Newtonian mechanics.

I. INTRODUCTION

In trying to choose a text for an intermediate mechanics course I was struck by how often I came across what I consider to be a completely erroneous interpretation of the first two of Newton's laws of motion. One encounters statements such as "Thus the First and Second Laws are not really 'laws' in the usual sense; rather, they may be considered *definitions*" (my emphasis).[1] A more extreme version of this position is the oft-repeated comment of Sir Arthur Eddington to the effect that all the first law says is that "every particle continues in its state of rest or uniform motion in a straight line except insofar as it doesn't."[2] Often coupled with such an interpretation is the equally erroneous, in my opinion, statement that the first law is a special case of the second law.

One reason why I would argue that the first two laws of motion should not be taken to be definitions is that they are poor definitions. In order to implement them it is necessary that one know what is a straight line, what is uniform motion (or rest), and what is mass. Although Newton assumed that these notions were obvious, they are in fact far from being so. To define a straight line one might, for example, introduce the notion of a rigid body. In doing so, however, one encounters many difficulties. How does one know that the body is rigid? How does one know that its length is constant in time? While it is in principle possible to deal with these objections, the complexities introduced as a consequence are completely unnecessary. As I will argue below, such complex physical systems as rigid rods are not needed for the formulation of the foundations of mechanics and, indeed, only find their appropriate description after such a foundation has been laid.

The main reason, however, for rejecting the interpretation of the first two laws as definitions is that such an interpretation misses the essential physics contained in these two laws. It also, incidentally, obscures an understanding of the transition from Newtonian physics to special and general relativity. And, in addition, it overlooks the fact that Newton was quite explicit in the *Principia* in distinguishing between definitions and laws. Unfortunately, his definition of force,

> An impressed force is an action exerted upon a body in order to change its
> state either of rest or of moving uniformly forward in a straight line

and his statement of the first law

> Every body continues in its state of rest or of uniform motion in a straight line, except in so far as it it compelled by forces to change that state

appear to be quite similar in content although the definition is a sufficient statement concerning the role of a force in changing the state of rest or uniform motion of a body while the first law is a necessary statement.

In Sec. II I will argue that Newton's first law asserts the existence of an ensemble of trajectories in a four-dimensional space, called here straight lines or free-body trajectories. These trajectories are the straight lines of Newton's

