compatible microcomputers. Copies will be sent to interested parties who send voluntary contributions to cover the cost of floppies and postage.

[1]B. C. Reed, "Linear least-squares fits with errors in both coordinates," Am. J. Phys. **57**, 642–646 (1989); "Erratum," Am. J. Phys. **58**, 189 (1990).

[2]D. York, "Least-squares fitting of a straight line," Can. J. Phys. **44**, 1079–1086 (1966).

[3]M. Lybanon, "A better least-squares method when both variables have uncertainties," Am. J. Phys. **52**, 22–26 (1984) and references therein; see also J. M. Pasachoff, "Applicability of least-squares formula," Am. J. Phys. **48**, 800 (1980) for more references. However, the citation by Pasachoff to F. H. Seares is incorrect: The page numbers should be 255 to 263.

[4]J. H. Williamson, "Least-squares fitting of a straight line," Can. J. Phys. **46**, 1845–1847 (1968).

[5]K. Pearson, "On lines and planes of closest fit to systems of points in space," Philos. Mag. **2**, 559–572 (1901).

[6]M. O'Neill, I. G. Sinclair, and F. J. Smith, "Polynomial curve fitting when abscissas and ordinates are both subject to error," Comput. J. **12**, 52–56 (1969).

[7]D. R. Powell and J. R. Macdonald, "A rapidly convergent iterative method for the solution of the generalized nonlinear least-squares problem," Comput. J. **15**, 148–155 (1972); "Errata," Comput. J. **16**, 51 (1973).

[8]D. R. Barker and L. M. Diana, "Simple method for fitting data when both variables have uncertainties," Am. J. Phys. **42**, 224–227 (1974).

[9]W. H. Southwell, "Fitting data to nonlinear functions with uncertainties in all measurement variables," Comput. J. **19**, 69–73 (1976).

Direct numerical integration of the radial equation

Frank Rioux

Department of Chemistry, Saint John's University, Collegeville, Minnesota 56321

(Received 22 March 1990; accepted for publication 15 May 1990)

Several articles have appeared in the Journal[1–7] describing simple algorithms for the numerical integration of Schrödinger's equation. Several well-known textbooks also discuss numerical integration briefly.[8–10]

When spherical coordinates are used the radial part of the Schrödinger equation (in atomic units) becomes

$$R''(r) + (2/r)R'(r) + \{2\mu[E - V(r)] - l(l+1)/r^2\}R(r) = 0. \quad (1)$$

It is customary in most numerical treatments to make the substitution, $P(r) = rR(r)$ to reduce the radial equation to a simpler form before integrating,

$$P''(r) + \{2\mu[E - V(r)] - l(l+1)/r^2\}P(r) = 0. \quad (2)$$

The disadvantage of this approach is that $P(r)$ and not the radial wave function is displayed. The purpose of this note is to describe a simple numerical algorithm that allows direct integration of the radial equation.

The first and second derivatives in Eq. (1) are approximated by the following finite differences,

$$R'(r) = [R(r+\delta) + R(r-\delta)]/2\delta, \quad (3)$$

$$R''(r) = [R(r+\delta) - 2R(r) + R(r-\delta)]/\delta^2. \quad (4)$$

Substitution of Eqs. (3) and (4) into Eq. (1) yields after rearrangement,

$$R(r+\delta) = \{2R(r) + [l(l+1)/r^2 - 2\mu(E - V(r))]R(r)\delta^2 - (1 - \delta/r)R(r-\delta)\}/(1 + \delta/r). \quad (5)$$

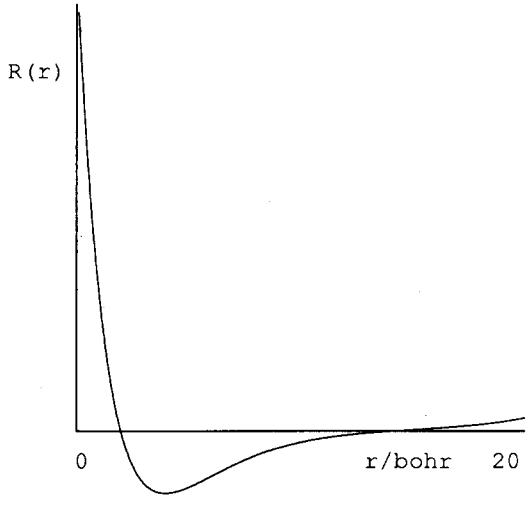

Fig. 1. Finding the solution for the 2*s* state; energy guess = −0.124 hartrees.

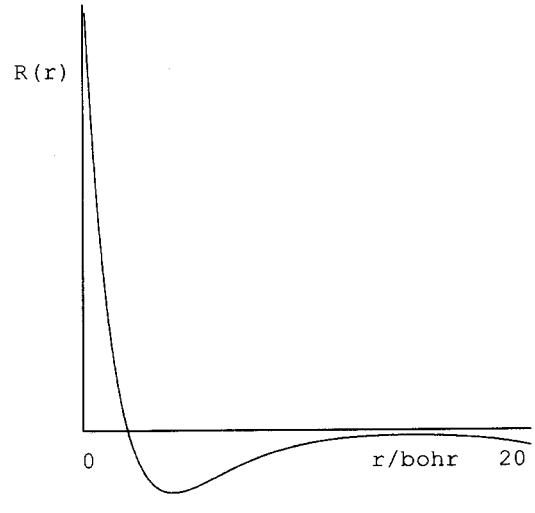

Fig. 2. Finding the solution for the 2*s* state; energy guess = −0.126 hartrees.

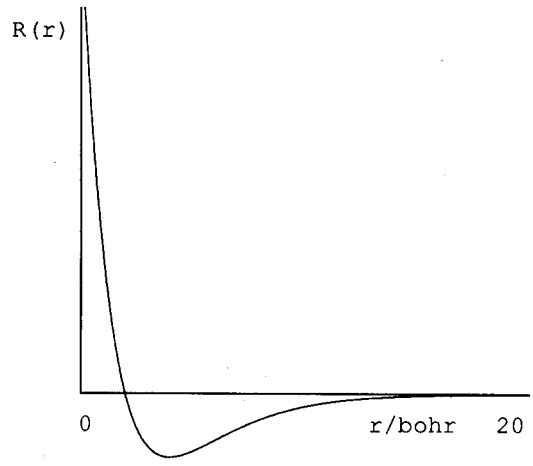

Fig. 3. Finding the solution for the $2s$ state; energy guess = -0.125 hartrees.

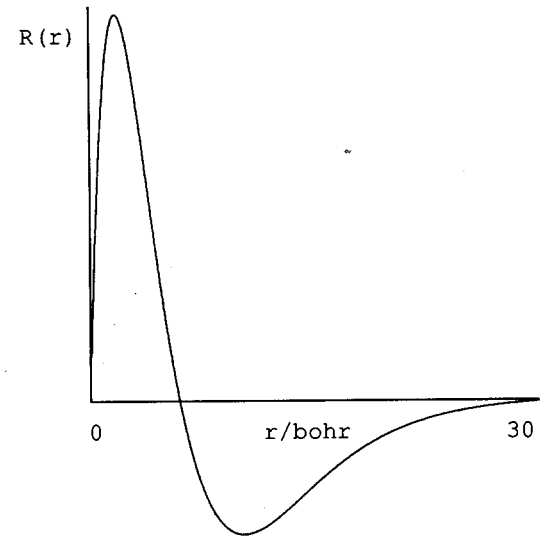

Fig. 5. The radial wave function for the $3p$ state obtained with an energy guess of -0.0555 hartrees.

The left boundary condition is used to obtain values for $R(r-\delta)$ and $R(r)$. A guess for E allows the generation of a wave function that can be displayed graphically on a monitor. If the right boundary condition is satisfied the energy guessed is an eigenvalue. If the right boundary condition is not satisfied another guess for the energy is made. It is rather easy to bracket the correct energy and move quickly to a solution.

Results using this algorithm are displayed in the accompanying figures. In atomic units the energy eigenvalues for the hydrogen atom are $-0.5/n^2$. Figures 1–3 illustrate the solution and two near misses for the hydrogen $2s$ state. It demonstrates that the algorithm is sufficiently accurate to be useful in applications with undergraduates. Figures 4 and 5 show solutions for the $3s$ and $3p$ states. The solutions obtained with this algorithm can be compared directly with textbook representations that are generated by plotting the analytical solutions.

One of the important advantages of numerical integration techniques is the ease with which one can move from one problem to another. For example, by changing the line of code containing the potential energy, the same program can be used for the hydrogen atom, the particle in the spherical potential well, the three-dimensional isotropic oscillator, the quark–antiquark interaction in charmonium, etc. In addition to demonstrating solutions for the traditional problems, the numerical approach facilitates the study of unusual potentials for which the analytical solutions are unknown or unavailable.

In summary, a simple and accurate algorithm for the numerical integration of the radial equation has been presented. It is suitable for use in undergraduate courses that cover quantum mechanics at an introductory or intermediate level. In addition to simplicity and accuracy it has the advantage of generating the radial wave function directly.

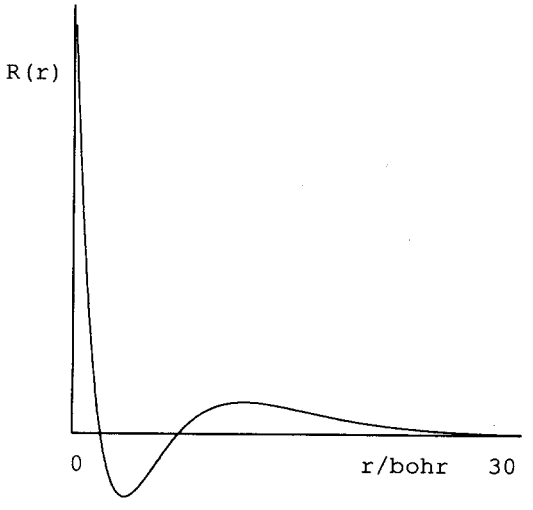

Fig. 4. The radial wave function for the $3s$ state obtained with an energy guess of -0.0555 hartrees.

[1]J. R. Merrill and G. P. Hughes, "Computer solutions to some simple one-dimensional Schrödinger equations," Am. J. Phys. **39**, 1391–1393 (1971).
[2]J. R. Merrill, "Introductory quantum mechanics with a computer," Am. J. Phys. **40**, 138–143 (1972).
[3]P. C. Chow, "Computer solutions to the Schrödinger equation," Am. J. Phys. **40**, 730–734 (1972).
[4]J. S. Bolemon, "Computer solutions to a realistic 'one-dimensional' Schrödinger equation," Am. J. Phys. **40**, 1511–1517 (1972).
[5]D. C. Griffin and J. B. McGhie, "General, interactive computer program for the solution of the Schrödinger equation," Am. J. Phys. **41**, 1149–1155 (1973).
[6]J. R. Merrill, "Introductory scattering theory with a computer," Am. J. Phys. **41**, 1156–1159 (1973).
[7]J. S. Bolemon and D. J. Etzold, "Enriching elementary quantum mechanics with the computer: Self-consistent field problems in one dimension," Am. J. Phys. **42**, 33–42 (1974).
[8]C. W. Sherwin, *Quantum Mechanics* (Holt, Rinehart and Winston, New York, 1959), Chap. 3.
[9]R. M. Eisberg and R. Resnick, *Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles* (Wiley, New York, 1985), 2nd ed., Appendix G.
[10]A. P. French and E. F. Taylor, *An Introduction to Quantum Physics* (Norton, New York, 1978), pp. 174–184, 216–220.