PHYSNET

MISN-0-253

SCHRÖDINGER EQUATION BOUND STATES

≡ Bound−State K's at zeros of A

SCHRÖDINGER EQUATION BOUND STATES
by
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1. Introduction and Overview

2. Preparing for Numerical Solution

3. Procedure for Numerical Solution

Project PHYSNET Physics Bldg. Michigan State University East Lansing, MI

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Title: **Schrödinger Equation Bound States**

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Length: 1 hr; 28 pages

Input Skills:

1. Solve the zero angular momentum radial Schrodinger equation numerically for given negative energies, using any given potential energy function (MISN-0-245).
2. Describe how the normalizability condition causes quantization of energy (MISN-0-245).

Output Skills (Knowledge):

K1. Show that zero-angular-momentum bound state solutions to the Schrödinger equation have the form: $u_0(r, K) = A(K)e^{Kr} + B(K)e^{-Kr}$ in all regions where the potential energy is constant, but not elsewhere.

K2. Show that bound states can only occur where $A(K) = 0$.

K3. Describe a method of locating all Schrödinger equation bound states in a given energy range for a given potential energy function.

Output Skills (Project):

P1. Choose a finite-range Schrodinger-equation potential and find all bound states within a self-chosen energy range. Demonstrate that all such states have been found. (See this module's *Local Guide* for how to obtain credit for this module.)

External Resources (Required):

1. A computer running Quick Basic (QBASIC).

SCHRÖDINGER EQUATION BOUND STATES

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1. Introduction and Overview

1a. Finding All Bound States Can Be Important. It is all very well to be able to use numerical techniques to find some of the bound states of a particular potential, but there are occasions where one would like to be sure of finding all of a potential energy function's bound states. For example, it can easily happen that adjustment of a potential-function parameter, in order to match the energy of a real-life bound state, results in a large energy shift for another observed bound state. Another example is the case where nature shows only one bound state for a particular system, yet a presumably applicable potential function produces two or more bound states. Thus one may need to locate all bound states of any given potential in order to make a complete comparison to data.

1b. Bound State: Increasing Exponential is Missing. Bound states occur only at isolated energy values because those are the only values where an exponentially-increasing part of the solution vanishes. Except at such energies Schrödinger equation solutions become rising exponentials at large radius as shown in Figure 1. For such cases the solution cannot be normalized to unity. That is, the condition that the bound
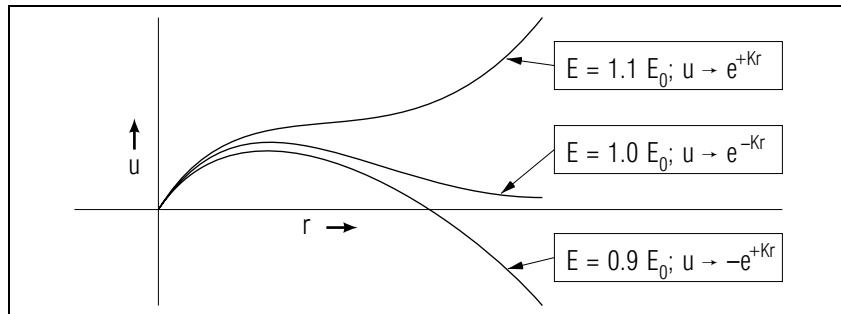
Figure 1. Hydrogen atom wave functins for 3 energies near the ground state energy E_0. A non-linear scale has been used.
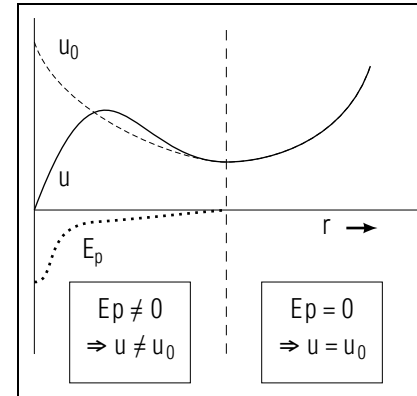
Figure 2. Wave function inside and outside a potential.

particle has 100% probability of being found somewhere in all of space,

$$1.00 = \int_0^\infty |u_{BS}(r)|^2 dr \,,$$

cannot be satisfied if u has a large-radius behavior like either $(+e^{Kr})$ or $(-e^{Kr})$ because then the integral will always diverge (be infinite). The problem is to find all of the discrete energies at which the exponentially-increasing part of the solution vanishes.

1c. The "Outside" Solution. In any region "outside" a potential, meaning in a region where the potential energy Ep is zero or negligibly small, the solution to the zero-angular-momentum Schrödinger equation is:

$$u_0 = Ae^{Kr} + Be^{-Kr} \;;\; \text{Help: [S-1]}$$

where A and B are functions of K but not of radius. This solution can be easily verified by direct substitution into a potential-less Schrödinger equation, along with the identification of K:

$$E = -\hbar^2 K^2/2m \;;\; \text{Help: [S-1]}$$

Notice that, if A is not zero, the A term will always win out over the B term for large enough radius (see Fig. 2). That is why the solution always increases exponentially for large radius - except at those precise values of K, hence of energy, where $A(K)$ is precisely zero.

1d. Findinq the Zeros of $A(K)$. The problem of finding the bound state energies reduces to finding the zeros of A, which is easily accomplished by plotting A vs K on a graph. A curve is obtained by numerically solving the Schrödinger equation at each of a number of K-values
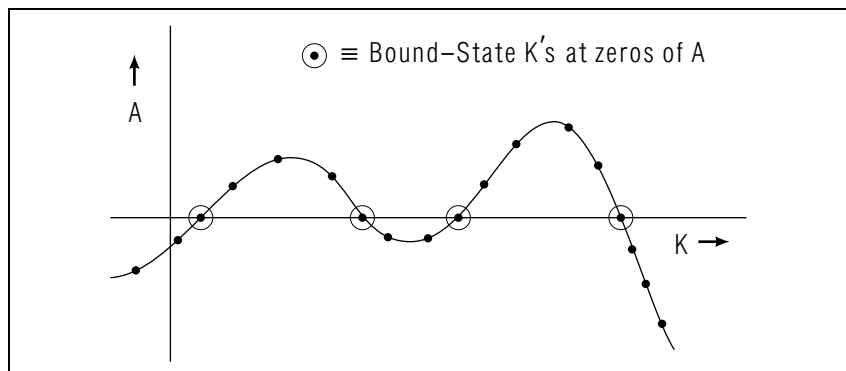
Figure 3. Locating the zeros of the exponentially-rising solution.

(energies). Then A is determined at each energy from the solution values at two different radii outside the potential:

$$u_1 \equiv u(r_1) = Ae^{Kr_1} + Be^{-Kr_1}$$
$$u_2 \equiv u(r_2) = Ae^{Kr_2} + Be^{-Kr_2} \quad (1)$$

These two equations in two unknowns can be easily solved for A. *Help: [S-2]*

1e. An Iterative Homing Procedure. Once the bound state energies have been fairly well delineated, an iterative automatic homing procedure can be used to find precision values for both the energy and wave function (solution "u"). There are a number of such procedures.[1]

2. Preparing for Numerical Solution

2a. Simplifying the Schrödinger Equation. Prior to numerical work we can simplify the Schrödinger equation by scaling its energies relative to a convenient radius scale. That is, we can first choose an appropriate unit of radius for graph plotting or other purposes, such as Bohr radius, fm, or whatever, then use a new measure of radius relative to those units:

$$R \equiv r/r_0.$$

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[1]See, for example, "An Automatic Variational Method for Schrödinger-Equation Bound States" (MISN-0-265, UC) and "Automatic Difference-Equation Methods for Schrödinger Bound States" (MISN-0-245, UC).

To simplify the Schrödinger equation we must choose an energy scale E_0, defined in terms of r_0 by

$$E_0 \equiv \hbar^2/(2mr_0^2), \quad (2)$$

and use new measures of energy which are relative to those units:

$$\epsilon \equiv E/E_0 \ ; \epsilon_p \equiv E_p/E_0.$$

Then the Schrödinger equation can be written simply:

$$d^2u/dR^2 = [\epsilon_p(R) - \epsilon]u. \ \textit{Help: [S-3]} \quad (3)$$

This form is easier to use in numerical calculations because it has fewer symbols to be programmed. Its "outside" ($\epsilon_p = 0$) solution is:

$$u_0 = Ae^{\kappa R} + Be^{-\kappa R}; \ \kappa \equiv \sqrt{-\epsilon}. \ \textit{Help: [S-4]} \quad (4)$$

2b. Modifications for an Energy Shift. The Schrödinger equation depends only on the difference of energies [see Eq. (3) above], so a constant can be added to each energy without altering the solution. This is sometimes desirable for making correspondence with other calculations. For example, the harmonic oscillator potential must usually be shifted in energy in order to match its minimum to that of a particular potential it is being used to approximate.[2] In any case, with an energy shift ϵ_c we can define new energy variables:

$$\epsilon'_p \equiv \epsilon_p + \epsilon_c \ ; \epsilon' \equiv \epsilon + \epsilon_c.$$

Then Eqs. (3) and (4) become:

$$d^2u/dR^2 = [\epsilon'_p(R) - \epsilon']u, \quad (5)$$

$$u_0 = Ae^{\kappa' R} + Be^{-\kappa' R}; \ \kappa' \equiv \sqrt{\epsilon_c - \epsilon'}. \ \textit{Help: [S-5]} \quad (6)$$

2c. Example: Cut-Off Hydrogen Atom Potential. An easily checked result can be obtained for the hydrogen atom, but with its Coulomb potential set equal to zero beyond some "cut-of" radius r_c as shown in Fig. 4. Then we only need go a short distance beyond r_c in order to pick up $u(r_l)$ and $u(r_2)$. The value of r_c can be chosen as small as 3 Bohr radii tor the ground state, while at least 7 Bohr radii of potential

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[2]See "Quantized Small Oscillation Technique" (MISN-0-264, UC)
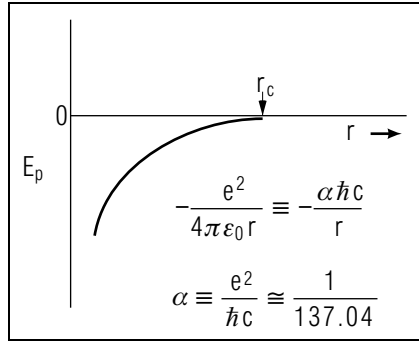
Figure 4. A cut-off potential.

is needed to produce the first excited state. A convenient radial unit to use[3] is the Bohr radius:

$$r_0 \equiv \hbar c/(\alpha mc^2) \simeq 0.53 \text{nm} \,. \tag{7}$$

Substituting Eq. (7) into Eq. (2) the energy-scale parameter is:

$$E_0 \equiv \alpha^2 mc^2/2 \,. \tag{8}$$

This is just the negative of the atom's ground state energy! Thus the scaled potential energy function is:

$$e_p(R) = -2/R \,.$$

2d. Cut-Off Radial Oscillator. A widely applicable and easily checked potential energy function is that of the radial harmonic oscil-

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[3] See Sect. 2a

Figure 5. The cut-off oscillator well.
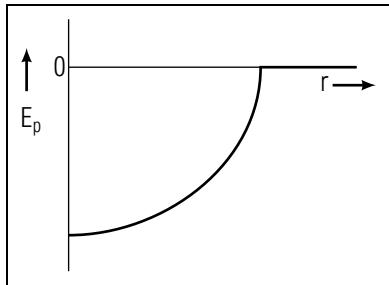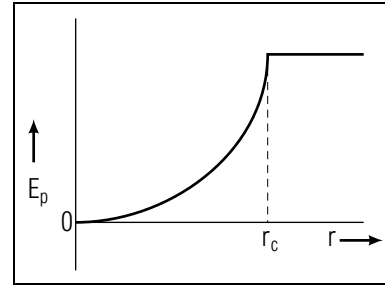
Figure 6. The well of Fig. 5 shifted upward by $kr_c/2$.

lator:[4]

$$E_p(r) = kr^2/2 \,. \tag{9}$$

Its energy levels are given by :

$$E_n = h\nu_0(2n + \frac{3}{2}) \; : n = 0, 1, 2, 3, \dots \; ; 2\pi\nu_0 \equiv \sqrt{k/m} \,.$$

In quantum phenomena the potential is usually better represented by the form (see Fig. 5):

$$r \leq r_c : \quad E_p(r) = \frac{1}{2}k(r^2 - r_c^2) \,,$$
$$r \geq r_c : \qquad E_p(r) = 0 \,.$$

However, it is customary to quote harmonic oscillator solutions in the form of Eq. (9) and then let them be subsequently adjusted to the requirements of particular applications. We accomodate to that convention by shifting our energies upward by $kr_c/2$ (see Fig. 6). Our new energies are:

$$r \leq r_c : \quad E_p' = kr^2/2 \,,$$
$$r \geq r_c : \quad E_p' = kr_c^2/2 \,.$$

We then define scale factors:[5]

$$r_0 \quad \equiv \quad (\hbar/2\pi\nu_0 m)^{1/2} \,,$$
$$E_0 \quad \equiv \quad \hbar^2/2mr_0^2 = h\nu_0/2 \,.$$

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[4] See: "Simple Harmonic Motion II" (MISN-0-26), "Small Oscillation Technique" (MISN-0-28), and "Quantized Small Oscillation Technique" (MISN-0-264).
[5] See Sect. 2a
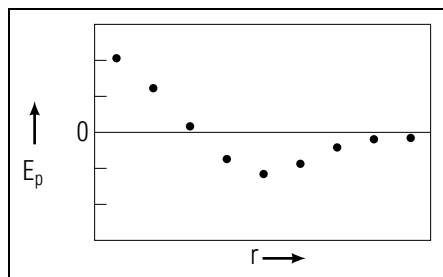
Figure 7. Numerical solution for the wave function.

and obtain a simplified Schrödinger equation:

$$R \le R_c : d^2U/dR^2 = (R^2 - \epsilon')u \,,$$
$$R \ge R_c : d^2U/dR^2 = (R_c^2 - \epsilon')u \,,$$
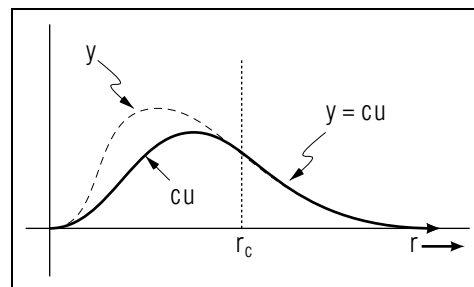
where:

$$R \equiv r/r_0 \,,$$
$$\epsilon' \equiv E'/E_0 \,.$$

2e. Dealing With Numerical Potentials. Sometimes the potential energy function is known only at a discrete number of radial points (see Fig. 7), whether from experiment or theory, so interpolative techniques must be used in order to solve the Schrödinger equation. One method is to fit all of the potential energy values with a combination of phenomenological functions. After adjustment of the functions' parameters for a sufficiently precise fit, the resulting potential energy function can be used directly in the computer technique normally used with formal potential energy functions. Another method is to use a standard computer "Table Look-Up" subroutine with, say, automatic quadratic interpolation. Such a subroutine must be given a table of potential energy values and a table of corresponding radii. Upon sending the routine a radius, it fits the three nearest-radius values with a quadratic, then evaluates the quadratic at the desired radius. Finally, some investigators prefer to fit different regions of the potential energy numbers with separate functions and then branch appropriately in the various regions of the numerical solution.

3. Procedure for Numerical Solution

3a. Finding the "Outside" Wave Function. In general, the wave function outside the potential is found numerically by use of a computational algorithm. A common example of such an algorithm, specifically

Figure 8. Joining the "inside" and "outside" wave functions.

applicable to the present case, is given elsewhere.[6] A saving in computation time can be gained in the present case where we only need the wave function outside the potential. In that region the algorithm's primary solution function $y(R)$ is simply proportional to the $u(R)$ we seek (see Fig. 8):

$$\text{"outside"} : y(R) = c\,u(R)$$

Now, any constant times a solution is also a solution so y itself is a solution in the outside region. Thus we merely solve for y and call its values, at two outside radii, u_1 and u_2. We have made available a computer programs to automatically get y at two such points.[7]

3b. Finding κ for $e^{\pm \kappa R}$. No matter what potential has been used, one must calculate A by comparing the "outside" solution y to:

$$y_0(R) = Ae^{\kappa R} + Be^{-\kappa R} \,.$$

This means finding y at two outside net-points and using the two equations to eliminate B and solve for A. The values of κ can be easily determined by putting the above form into the Schrödinger equation for u_0. The result is:

$$\kappa = \sqrt{\epsilon_p(\text{outside}) - \epsilon} \,, \ \textit{Help: [S-4]}$$

where $\epsilon_p(\text{outside})$ is usually zero for negative ϵ's and a positive constant for positive ones.[8]

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[6]See "Numberical Demonstration of Energy Quanitzation for Atomic Hydrogen" (MISN-0-245, UC).
[7]See Appendix A
[8]See Sect. 2.

3c. Finding A for Each Energy.　　Values of y at two outside radii are used to find A:

$$A = \frac{y_2 e^{-\kappa R_1} - y_1 e^{-\kappa R_2}}{e^{\kappa(R_2-R_1)} - e^{-\kappa(R_2-R_1)}} , \ Help: [S\text{-}2]$$

One can use this formula with a pre-made program (see Appendix A), for a computer, or perform the calculation manually. Repeating this calculation for a number of different ϵ values, the A vs. ϵ curve can be plotted and sketched-in smoothly. To obtain high accuracy the region around a zero of A can be blown up, in the photographic sense, until the A points are highly linear. Graphical or numerical interpolation is then very accurate *Help: [S-6] Help: [S-7]*. Finally, the bound state energies can be put back into the Schrödinger Equation program and the wave function tails examined visually as a check.

NOTE: Be sure to include only one **FUNCTION** ep, that for the appropriate potential, in your program at a time.

3d. Precision Energies and Wave Functions.　　Once the bound states of a given potential have been located, we recommend switching to methods which automatically "home in on" solutions to produce precise energies and precise and/or functional representations of the wave functions. Such methods are given elsewhere.[9]

Acknowledgments

A. Qbasic to Calculate Bound States

```
'PROGRAM BOUND 9/28/99

DECLARE SUB NPUT ()
DECLARE SUB INIT ()
```

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[9] See "An Automatic Variational Method for Schrödinger-Equation Bound States" (MISN-0-265) and "Automatic Difference-Equation Methods for Schrödinger-Equation Bound States" (MISN-0-245).

```
DECLARE SUB INITIAL ()
DECLARE SUB GETA ()
DECLARE SUB TPUT ()
DECLARE SUB ITERATE ()

COMMON SHARED delta!, rc!, emin!, emax!, eino%
COMMON SHARED e!
COMMON SHARED de!, nept%
COMMON SHARED yi!, ypi!, ri!, rs!
COMMON SHARED yf!, ypf!, rf!, rpf!, epf!
COMMON SHARED a!

DECLARE FUNCTION ep! (ep1!, ep2!)
DECLARE FUNCTION yplus! (yp1!, yp2!, yp3!, yp4!, yp5!)

'Begin Main Program

CALL NPUT
CALL INIT

FOR ne% = 1 TO nept% STEP 1
    ' e! = The Total Energy at the Interval Points
    e! = emin! + (ne% - 1) * de!
    CALL INITIAL
    CALL ITERATE
    CALL GETA
  CALL TPUT
NEXT ne%

'End Main Program

SUB NPUT

    ' delta! = Radial Stepping Increment
    ' rc! = Cut-Off Radius
    ' emin! = Minimum Energy Desired
    ' emax! = Maximum Energy Desired
    ' eino! = # of Energy Sub-Int. Desired in (emin!,emax!)

    INPUT "Enter the Radial Stepping Increment: ", delta!
    INPUT "Enter the Cut-Off Radius         : ", rc!
```

      INPUT "Enter␣the␣Minimum␣Energy␣Desired␣␣␣:␣", emin!
      INPUT "Enter␣the␣Maximum␣Energy␣Desired␣␣␣:␣", emax!
      INPUT "Enter␣the␣Number␣of␣Sub−Intervals␣␣:␣", eino%

END SUB

SUB INIT

      ' de! = Energy Increment
      ' nept = Number of Energy Points Desired

      nept% = eino% + 1
      de! = 0
      IF (eino% <> 0) **THEN**
          de! = (emax! − emin!) / eino%
      END IF

END SUB

SUB INITIAL

      ' yi! = Y − Wave Function at the Origin
      ' ypi! = Y − Wave Function at the First Net Point
      ' ri! = Radius for y
      ' rs! = Maximum Radius

      rs! = rc! + (2 ∗ delta!)
      yi! = 0
      ypi! = 1
      ri! = 0

END SUB

SUB ITERATE

      ' yf! = Y − Wave Function at Next−To−Final Radius
      ' ypf! = Y − Wave Function at Final Radius
      ' rf! = Next−To−Final Radius
      ' rpf! = Final Radius
      ' epf! = Potential Energy at Final Radius,
      '   Same Units as Total Energy e!

      y! = yi!
      yp! = ypi!
      r! = ri!

      DO

          r! = r! + delta!
          ym! = y!
          y! = yp!
          ept! = ep!(r!, rc!)
          yp! = yplus!(delta!, e!, ept!, ym!, y!)

      LOOP WHILE (r! < rs!)

      yf! = y!
      ypf! = yp!
      rf! = r!
      rpf! = r! + delta!
      epf! = ep!(r!, rc!)

END SUB

SUB GETA

      ' a! = Coefficient of Rising Exponential

      ak! = **SQR**(epf! − e!)
      a1! = **EXP**(ak! ∗ rf!)
      a2! = **EXP**(ak! ∗ rpf!)
      a! = (ypf! / a1! − yf! / a2!) / (a2! / a1! − a1! / a2!)

END SUB

SUB TPUT

      PRINT
      PRINT USING "D=##.######"; delta!;
      PRINT USING "␣RC=##.##"; rc!;
      PRINT USING "␣E=##.######"; e!;
      PRINT USING "␣A=##.######"; a!

END SUB

FUNCTION yplus! (yd!, ye!, yep!, yym!, yy!)

     'Calculates Y − Wave Function at Next Radius

     dst! = yd! ∗ yd! ∗ (yep! − ye!) / 12
     yplus! = (2 + 10 ∗ dst!) ∗ yy! / (1 − dst!) − yym!

END FUNCTION

FUNCTION ep! (er!, erc!)

'Calculates Potential Energy for H Atom, Bohr Radius Units

    ep! = 0
    IF (er! < erc!) **THEN**
        ep! = −2 / er!
      END IF

END FUNCTION

FUNCTION ep! (er!, erc!)

'Calculates Potential Energy for Radial Harmonic Oscilator
'Radius Units are hbar∗∗(0.5)/(k∗mass)∗∗(0.25)
'Energy Units are h∗nu/2

     IF (er! <= erc!) **THEN**
        ep! = er! ∗ er!
     END IF
     IF (er! > erc!) **THEN**
        ep! = erc! ∗ erc!
     END IF

END FUNCTION

B. Sample Results: Hydrogen Atom

Hydrogen Atom Potential:

Please Enter the Radial Stepping Increment: .1
Please Enter the Cut−Off Radius   : 3
Please Enter the Minimum Energy Desired : −1.1
Please Enter the Maximum Energy Desired : −0.9
Please Enter the Number of **Sub**−Intervals : 2

D= 0.100000 RC= 3.00 E=−1.100000 A= 0.063856

D= 0.100000 RC= 3.00 E=−1.000000 A= 0.015900

D= 0.100000 RC= 3.00 E=−0.900000 A=−0.040630

C. Sample Results: Harmonic Oscillator

Harmonic Oscilator Potential:

Enter the Radial Stepping Increment: .1
Enter the Cut−Off Radius   : 3
Enter the Minimum Energy Desired : 2
Enter the Maximum Energy Desired : 4
Enter the Number of **Sub**−Intervals : 2

D= 0.100000 RC= 3.00 E= 2.000000 A= 0.016358

D= 0.100000 RC= 3.00 E= 3.000000 A=−0.000009

D= 0.100000 RC= 3.00 E= 4.000000 A=−0.016484

SPECIAL ASSISTANCE SUPPLEMENT

S-1   *(from Text 1b.)*

$$u_0 = A(K)e^{Kr} + B(K)e^{-Kr} \,.$$

The Schrodinger Equation:

$$-\frac{\hbar^2}{2m}\frac{d^2 u_0}{dr^2} + E_p\, u = E\, u$$

In any region where Ep is negligible:

$$-\frac{\hbar^2}{2m}\frac{d^2 u_0}{dr^2} = E\, u_0 \,. \quad (a)$$

Now:

$$\frac{d^2}{dr^2}(Ae^{Kr} + Be^{-Kr}) = K^2(Ae^{Kr} + Be^{-Kr}) \,,$$

so, putting into (a),

$$-\frac{\hbar^2 K^2}{2m}\, u = E\, u \,;$$

$$-\frac{\hbar^2 K^2}{2m} = E \,.$$

Both sides are constant hence this equation defines K. Thus, for $E_p = 0$,

$$u_0 = Ae^{Kr} + Be{-}Kr \,,$$

provided we calculate K from:

$$K \equiv \frac{\sqrt{-2mE}}{\hbar} \,.$$

S-2   *(from Text 1d, 3c.)*

$$u_1 \equiv Ae^{\kappa R_1} + Be^{-\kappa R_1} \quad ; \quad E_p(R_1) = 0$$
$$u_2 \equiv Ae^{\kappa R_2} + Be^{-\kappa R_2} \quad ; \quad E_p(R_2) = 0$$

1. Multiply the first equation (both sides) by $e^{-\kappa R_2}$.

2. Multiply the second equation by $e^{-\kappa R_1}$.

3. Subtract the two resulting equations.

4. Solve for A.

S-3   *(from Text 2a.)*

Schrödringer Equation: $-\frac{\hbar^2}{2m}\frac{d^2 u}{dr^2} + E_p\, u = E\, u \,. \quad (a)$

$$\frac{d^2 u}{dr^2} = \frac{d^2 u}{d(r_0 R)^2} = \frac{1}{r_0^2}\frac{d^2 u}{dR^2} \,. \quad (b)$$

The rest of the the derivation of involves no unusual techniques. *Help: [S-8]*

S-4   *(from Text 2a, 3b.)*

Translate *[S-1]* into the symbols of this section.

S-5   *(from Text 2b.)*

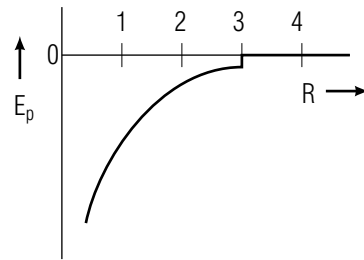"Outside" $(\epsilon_p' = \epsilon_c)$:

$$\frac{d^2 u}{dR^2} = (\epsilon_c - \epsilon')\, u_0 \,,$$

$$u_0 = Ae^{\kappa' R} + Be^{-\kappa' R} \,.$$

Following the same procedure as in *[S-3]* we get the result:

$$\epsilon_c - \epsilon' = (\kappa')^2 \,.$$

S-6   *(from Text 3c.)*

To the right is the Coulomb potential cut off at 3 Bohr radii. We found values for y_n and A, listed in the table below, using the third order Numerov method and these parameters:

$$\epsilon \equiv E/E_0 \ , \ \ R \equiv r/r_0 \,,$$
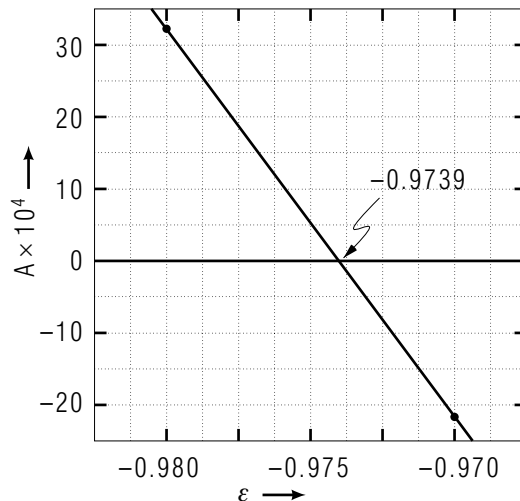
$$\delta \equiv \Delta/r_0 = 0.1 \,, \ y(0.1) = 1 \,.$$

ϵ	$y(3.2)$	$y(3.3)$	$A \times 10^4$
0.970	1.07942725	0.96843997	-21.13
0.975	1.14723425	1.04213642	5.94
0.980	1.21556178	1.11643747	32.79

We then plotted A vs. ϵ, as shown, and obtained:

$$\epsilon = -0.9739 \,.$$

Thus:

$$E = (-0.9739)(13.6\text{eV})$$
$$= -13.2\text{eV} \,.$$

This is not quite as strong binding as in the true hydrogen atom, but that was to be expected since we weakened the potential by cutting it off beyond 3 Bohr radii. For comparison, the no-cut-off solution ($R_c \rightarrow \infty$): $\epsilon = -1$, $u = Re^{-R}$. You can try these in the Schrödinger Equation (See *Text 2a, 2b*).

S-7   *(from Text 3c.)*
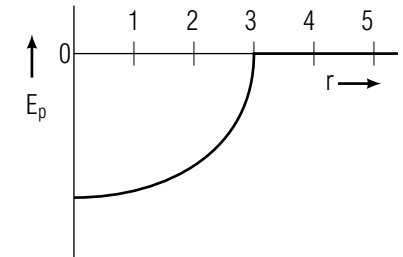
To the right is the Radial Harmonic Oscillator cut off at $R_c = 3$. Define:

$$E_0 \equiv \frac{h\nu_0}{2} \,,$$
$$2\pi\nu_0 \equiv \sqrt{k/m} \,,$$
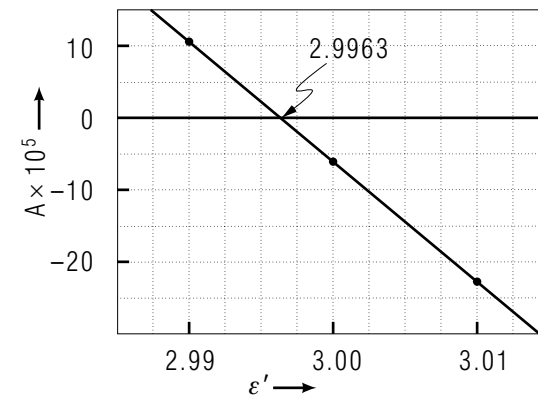$$R \equiv \sqrt{(mk)^{1/4}(\hbar)} \ r \,,$$
$$\epsilon \equiv (E + \frac{1}{2}kr_c^2)/E_0 \,.$$

The "outside" solution is:

$$u_0 = Ae^{\kappa R} + Be^{-\kappa R} \,, \ \text{with} \ \kappa \equiv \sqrt{R_c^2 - \epsilon'} \,.$$

Using $\delta \equiv \Delta/r_0 = 0.1$ and the third order Numerov, we find the results shown below:

Our value of $\epsilon'_0 = 2.9963$ is very close to the no-cut-off case where:

$$\epsilon'_0 = 3 \,; \ u_0 = Re^{-R^2/2} \,.$$

You can try these in the Schrödinger equation (See *Text 2a, 2c*).

S-8 *(from [S-3])*

1. Substitute (b) into (a) in *[S-3]*.

2. Multiply all terms of the equation by $(-2mr_0^2/\hbar^2)$.

3. Replace E_p and E and their multipliers by ϵ_p and ϵ respectively.

LOCAL GUIDE

Credit for this Module

As specified in this modules *ID Sheet*, specifically Output Skill P1, choose a finite range Schrödinger-equation potential, and locate all the bound states within a self-chosen energy range.

You may use the program included in this module, one of your own construction, or calculate by hand, relevant values. In any case you must provide:

1. A printout of the computer program used, either your own or the one included in this module, or sample of hand calculations. Your work may not include any part of the sample results included with the program in the Appendix.

2. An original graph illustrating coefficient A versus energy ϵ within your self-chosen range, noting that range and the particular Schrödinger-potential you have chosen. This graph must clearly illustrate all the bound states within the energy range. The bound state energies should be noted in a separate table.

3. The bound state solutions to the Schrödinger equation outside must be calculated and there behavior in all regions inside and outside the potential clearly displayed.

Bring all your original material, not a copy, with you to the exam room and check in as with any other exam. Answer any exam questions pertaining to the Knowledge Output Skills of the module.

The last "question" of the exam will direct you to hand in your original materials relating to the project. Your "answer" to this question should be a reference to your material which you should attach to your exam sheets, immediately following the answer sheets.

A lack of project originals will cause the grader to assign a grade of zero to the entire exam.

Now read all of this module's *Model Exam*.

MODEL EXAM

1. See Output Skill K1-K3 in your module's *ID Sheet*. Some or all of these skill may be tested in the actual exam.

Examinee:

On your computer output sheet(s):

  (i) Mark page numbers in the upper right corners of all sheets.

  (ii) Label all output, including all axes on all graphs.

On your Exam Answer Sheet(s), for each of the following parts of items (below this box), show:

  (i) a reference to your annotated output; and

  (ii) a blank area for grader comments.

When finished, staple together your sheets as usual, but include the original of your annotated output sheets just behind the Exam Answer Sheet.

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2. Using pre-prepared materials, show that you have found all bound states of the Schrödinger equation within a self-chosen energy range. Display the solutions for those bound states, clearly showing the decaying-exponential behavior outside the potential.

INSTRUCTIONS TO GRADER

If the student has submitted copies rather than originals of the computer output, state that on the exam answer sheet and **immediately stop grading the exam and give it a grade of zero.**

Brief Answers:

1.- 2. See this module's *text*.