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COMPUTATION OF S-STATE BINDING ENERGY AND WAVE FUNCTIONS IN A SAXON–WOODS POTENTIAL

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PROGRAM SUMMARY

Title of program: BSSW

Catalogue number: ABGL

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: IBM 370/155; *Installation*: University of Liege

Operating system: MVT-R20.7

Programming language used: FORTRAN IV (G)

High speed storage required: 1143 words.
No. of bits in a word: 32

Overlay structure: None

No. of magnetic tapes required: None

Other peripherals used: Card reader, line printer

No. of cards in combined program and test deck: 300

Card punching code: BCD

Keywords: Nuclear s-state, Woods–Saxon potential, Fox–Goodwin method, spectroscopic number, S-matrix.

Nature of the physical problem

The program computes the energy and the wave function of the s-state in a Saxon–Woods potential. It can also determine the well depth or radius which fits a given binding energy.

Method of solution

The S-matrix for negative energies is obtained analytically using a method given by Bencze [1]. The equation giving its poles is transformed into a real equation whose solutions are the bound state energies. The wave function is obtained by integrating the Schrodinger equation using the Fox–Goodwin method.

Restrictions on the complexity of the problem

Only s-states.

Typical running time

The running time is 0.2–0.3 sec for the bound state energy alone, 0.8–0.9 sec if the wave function is required.

Reference

[1] G. Bencze, Comment. Physico-Mathemat. 31 (1966) 1.

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LONG WRITE-UP

1. Introduction

The Woods–Saxon potential is widely used in nuclear physics to describe the bound and scattering states of various systems like neutron + nucleus, alpha particle + nucleus and now, ion + ion. The programs used up to now to compute the bound state energy and wave function match the integrated solutions of the Schrodinger equation starting from inside and from outside the well. This procedure requires a long time. In BSSW, the bound state energy is computed very fast (a fraction of second) using an analytical method for s-waves [1]. The wave function is obtained by integrating the Schrodinger equation using the Fox–Goodwin method. Besides its rapidity, the program offers some other advantages: *i*) it works very well for loosely bound states for which previous methods are often divergent. *ii*) it can easily be transformed into a subroutine which may be advantageously introduced in DWBA codes, when particles are transferred in s-states. *iii*) the program can also determine the well depth or the well radius which fits a given binding energy. In particular, it is very easy to find a depth corresponding to a critical potential, which is very difficult with previous methods. Those critical potentials are related with maxima in neutron strength functions [2].

2. Method of solution

It is easy to get an analytical solution for an s-wave using the method described by Bencze [1]. We only sketch the procedure. We start from the equation

$$\frac{d^2u}{dr^2} + \frac{2\mu}{\hbar^2}\left[-E_B + \frac{V_0}{1+e(r-R)/a}\right] u = 0 , \tag{1}$$

where μ is the reduced mass and E_B the binding energy. Introducing $b = \exp(-R/a)$ and $x = -b\,e^{r/a}$, and making the substitution

$$u(x) = x^{\lambda}\varphi(x) , \tag{2}$$

with

$$\lambda = ia\sqrt{(2\mu/\hbar^2)(V_0 - E_B)} \equiv i\Lambda , \tag{3}$$

we get

$$\left[x(1-x)\frac{d^2}{dx^2} + (2\lambda+1)(1-x)\frac{d}{dx} - (2\mu/\hbar^2)E_B a^2\right]\varphi = 0 . \tag{4}$$

The solution φ can be expressed as a linear combination of hypergeometrical functions. The condition $u(r=0) = 0$ completely determines the wave function except for a normalization constant. By looking at the asymptotic behaviour, it is easy to get the S-matrix [1]. For negative energies the zeros of the S-matrix are given by:

$$A - \frac{\Gamma(1+2i\Lambda)\,\Gamma(1+\kappa a - i\Lambda)\,\Gamma(\kappa a - i\Lambda)}{\Gamma(1-2i\Lambda)\,\Gamma(1+\kappa a + i\Lambda)\,\Gamma(\kappa a + i\Lambda)} = 0 , \tag{5}$$

and

$$A = [b/(1+b)]^{2i\Lambda}(1+b)^{2\kappa a}\,F(1-\kappa a+i\Lambda, -\kappa a+i\Lambda, 1+2i\Lambda, b/(1+b))/F(1+\kappa a-i\Lambda, \kappa a-i\Lambda, 1-2i\Lambda, b/(1+b)), \tag{6}$$

where $\kappa = \sqrt{(2\mu/\hbar^2)E_B}$ and F is the hypergeometric function. We are going to show that eq. (5), which apparently looks like a complex equation, is in fact equivalent to a real equation of one variable. Since $\Gamma(Z^*) = \Gamma^*(Z)$, it is

sufficient to show that $AA^* = 1$. Applying the relation [3]

$$F(\alpha, \beta, \gamma, Z) = \frac{\Gamma(\gamma)\,\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)}\,F(\alpha, \beta, \alpha+\beta-\gamma+1, 1-Z)$$

$$+ (1-Z)^{\gamma-\alpha-\beta}\,\frac{\Gamma(\gamma)\,\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha)\,\Gamma(\beta)}\,F(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1, 1-Z) \qquad (7$$

for both hypergeometric functions in (6), and taking the following relation into account:

$$F(\alpha^*, \beta^*, \gamma^*, Z^*) = F^*(\alpha, \beta, \gamma, Z), \qquad (8$$

we can show that

$$F(1-\kappa a+\mathrm{i}\Lambda, -\kappa a+\mathrm{i}\Lambda, 1+2\mathrm{i}\Lambda, b/(1+b)) = [1/(1+b)]^{2\kappa a}\,F^*(1+\kappa a-\mathrm{i}\Lambda, \kappa a-\mathrm{i}\Lambda, 1-2\mathrm{i}\Lambda, b/(1+b)). \qquad (9$$

Then, eq. (4) is equivalent to

$$\phi(\kappa) = 0, \qquad (10$$

with

$$\phi = -2\Lambda \ln [b/(1+b)] - 2\phi_0 + 2\phi_1 + 4\phi_2 + 2 \arctan(\Lambda/\kappa a), \qquad (11$$

and

$$\phi_0 = \arg F(1-\kappa a+\mathrm{i}\Lambda, -\kappa a+\mathrm{i}\Lambda, 1+2\mathrm{i}\Lambda, b/(1+b)), \quad \phi_1 = \arg \Gamma(1+2\mathrm{i}\Lambda), \quad \phi_2 = \arg \Gamma(\kappa a-\mathrm{i}\Lambda).$$

The function $\phi(\kappa)$ possesses interesting properties:

i) in practical cases, it is a monotonically decreasing function of κ. Indeed, it is easy to see that, in general, ϕ_0 is very small (because b is small), $-2\Lambda \ln [b/(1+b)] + \arctan(\Lambda/\kappa a)$ is always decreasing when κ increases, and ϕ_1 and ϕ_2 are also decreasing except for very small values of Λ;

ii) ϕ has a non-physical zero when $E_B = V_0$; by "non-physical" we mean that it does not correspond to a bour state. This is illustrated by fig. 1.

In order to solve numerically eq. (10), we proceed as follows. Starting from a given value of E_B (or V_0 or R), we make a linear extrapolation of the function ϕ, which has a root at $E_B = x$. At this value, we again do a linear extrapolation which gives a new value of x. The process is stopped when the difference between two successive values of x is less than the desired accuracy (ERR in the input data). This procedure is very fast in this problem because of the almost linear variation of the function $\phi(\kappa)$.

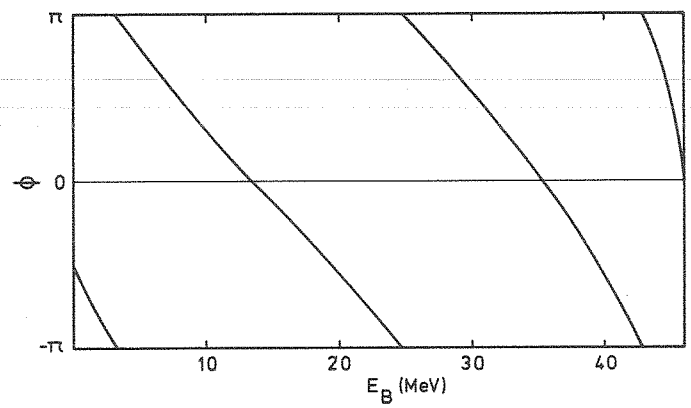

Fig. 1. Typical variation of the function ϕ versus E_B. The parameters are: $V_0 = 46$ MeV, $R = 4.534$ fm, $a = 0.62$ fm.

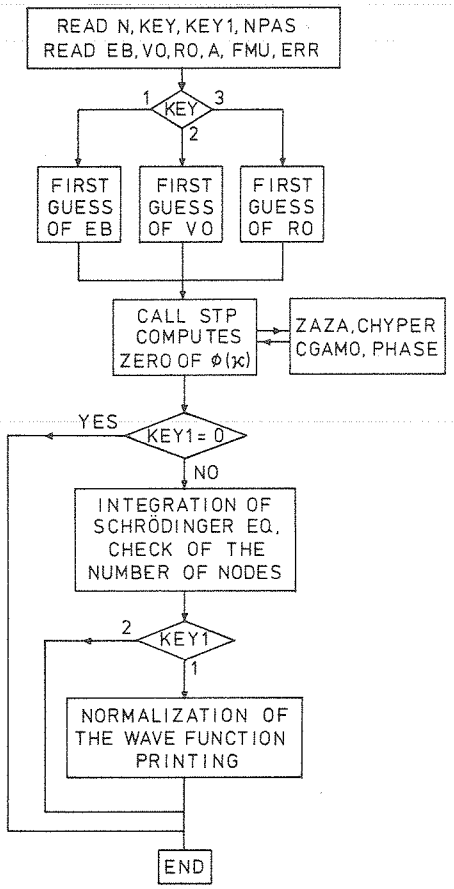

Fig. 2. General diagram.

3. Program structure

The general flow diagram is illustrated by fig. 2. The main program first reads the input data which are defined by the detailed comments in the source program. Then it makes a first estimate of the unknown parameter (E_B, V_0 or R), if it is not given in the input data.

The subroutine STP(V, A, FMU, ERR, KEY) computes the zero of the function ϕ by the procedure explained in the previous section. The computation of the function ϕ is done by the subroutine ZAZA(V0, R0, A, EB, FMU, ERR).

Following the value of the control data KEY1, the program stops or it integrates the Schrödinger equation in order to check the number of nodes of the wave function. A printing of the normalized wave function can also be obtained for a special value of KEY1.

The subroutine CHYPER(CA, CB, CC, CZ, EPS) computes the hypergeometric function $F(\alpha, \beta, \gamma, Z)$ for complex α, β, γ, Z with an accuracy less than or equal to EPS. The value of EPS assumed here (in subroutine ZAZA) is: EPS = 10^{-8}, but can be changed.

The subroutine CGAMO(CZ, EPS) computes the complex gamma function $\Gamma(Z)$ with an accuracy less than or equal to EPS.

Finally, the subroutine PHASE(Z) determines the phase of a complex number Z between $-\pi$ and π.

4. Input and output data

The input data (N, KEY, KEY1, NPAS, EB, V0, R0, FMU, ERR) are described by the comments in the source program.

The output data contain:

1. the starting values of E_B, V_0, R and a.
2. the intermediate values of E_B (or V_0 or R) which are obtained successively in the procedure of solving eq. (10).
3. the final values of E_B, V_0, R and a.
4. eventually one of the following two diagnostic messages:
   i) INCORRECT NUMBER OF NODES
   if, for instance, the 3s state is obtained instead of the 2s state. This message is followed by the effective number of nodes. The starting value of the unknown parameter must be changed.
   ii) UNBOUND LEVEL
   if the function ϕ has no root for E_B positive.
5. the values of the normalized wave function (for appropriate value of KEY1). They correspond to $r = n(\Delta r)$ with $n = 1, 2, \ldots,$ NPAS, and $\Delta r = (R_0 + 10a)/\text{NPAS}$.

5. Test runs

1. 2s state in ^{40}Ca. Parameters: $V_0 = 46$ MeV, $R = 4.534$ fm, $a = 0.62$ fm, $\mu = 0.9756$. The initial value for E_B is 20.4495 MeV. The required accuracy is 0.001 MeV. Values of the control data: $N = 2$, KEY = 1, KEY1 = 1 NPAS = 200.

2. Critical potential for the 4s state (around Tm). Parameters: $V_0 = 49$ MeV, $E_B = 0$, $a = 0.52$ fm, $\mu = 0.994$. The initial value of R is 7 fm. The required accuracy is 0.0001 fm. Values of the control data: $N = 4$, KEY = 3, KEY1 = 2, NPAS = 200.

References

[1] G. Bencze, Commentat. Phys. Math. 31 (1966) 1.
[2] A.E.S. Green, T. Sawada, D.S. Saxon, The Nuclear Independent Particle Model (Academic Press, New York 1069), ch. 4.
[3] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions (N.B.S., Washington 1965), ch. 15.

TEST RUN OUTPUT

FIRST TEST RUN

```
SEARCH OF THE BINDING ENERGY

STARTING VALUES EB= 20.449493  VO= 46.000000  RO=  4.533999  A=  0.620000

X1= 13.338008
X1= 13.423724
X1= 13.447281
 FINAL VALUES   EB= 13.446569  VO= 46.000000  RO=  4.533999  A=  0.620000

DISTANCE R     NORMALIZED WAVE FUNCTION

    0.5367E-01     0.3460E-01
    0.1073E 00     0.6904E-01
    0.1610E 00     0.1032E 00
    0.2147E 00     0.1369E 00
    0.2683E 00     0.1700E 00
    0.3220E 00     0.2023E 00
    0.3757E 00     0.2338E 00
    0.4294E 00     0.2642E 00
    0.4830E 00     0.2935E 00
    0.5367E 00     0.3215E 00
    0.5904E 00     0.3482E 00
    0.6440E 00     0.3732E 00
    0.6977E 00     0.3967E 00
    0.7514E 00     0.4184E 00
    0.8050E 00     0.4383E 00
    0.8587E 00     0.4563E 00
    0.9124E 00     0.4723E 00
    0.9661E 00     0.4863E 00
    0.1020E 01     0.4981E 00
    0.1073E 01     0.5078E 00
    0.1127E 01     0.5152E 00
    0.1181E 01     0.5204E 00
    0.1234E 01     0.5234E 00
    0.1288E 01     0.5241E 00
    0.1342E 01     0.5225E 00
    0.1395E 01     0.5186E 00
    0.1449E 01     0.5125E 00
    0.1503E 01     0.5042E 00
    0.1556E 01     0.4936E 00
    0.1610E 01     0.4810E 00
    0.1664E 01     0.4663E 00
    0.1717E 01     0.4495E 00
    0.1771E 01     0.4308E 00
    0.1825E 01     0.4103E 00
    0.1878E 01     0.3880E 00
    0.1932E 01     0.3641E 00
    0.1986E 01     0.3385E 00
    0.2039E 01     0.3116E 00
    0.2093E 01     0.2833E 00
    0.2147E 01     0.2538E 00
    0.2200E 01     0.2232E 00
    0.2254E 01     0.1917E 00
    0.2308E 01     0.1593E 00
    0.2361E 01     0.1263E 00
    0.2415E 01     0.9279E-01
    0.2469E 01     0.5887E-01
    0.2522E 01     0.2470E-01
    0.2576E 01    -0.9565E-02
    0.2630E 01    -0.4380E-01
    0.2683E 01    -0.7785E-01
    0.2737E 01    -0.1116E 00
    0.2791E 01    -0.1449E 00
```

```
0.2845E 01   -0.1776E 00
0.2898E 01   -0.2095E 00
0.2952E 01   -0.2407E 00
0.3006E 01   -0.2709E 00
0.3059E 01   -0.3001E 00
0.3113E 01   -0.3281E 00
0.3167E 01   -0.3548E 00
0.3220E 01   -0.3803E 00
0.3274E 01   -0.4043E 00
0.3328E 01   -0.4268E 00
0.3381E 01   -0.4478E 00
0.3435E 01   -0.4672E 00
0.3489E 01   -0.4850E 00
0.3542E 01   -0.5011E 00
0.3596E 01   -0.5156E 00
0.3650E 01   -0.5284E 00
0.3703E 01   -0.5395E 00
0.3757E 01   -0.5489E 00
0.3811E 01   -0.5567E 00
0.3864E 01   -0.5629E 00
0.3918E 01   -0.5675E 00
0.3972E 01   -0.5705E 00
0.4025E 01   -0.5721E 00
0.4079E 01   -0.5723E 00
0.4133E 01   -0.5711E 00
0.4186E 01   -0.5686E 00
0.4240E 01   -0.5649E 00
0.4294E 01   -0.5600E 00
0.4347E 01   -0.5542E 00
0.4401E 01   -0.5473E 00
0.4455E 01   -0.5396E 00
0.4508E 01   -0.5310E 00
0.4562E 01   -0.5218E 00
0.4616E 01   -0.5119E 00
0.4669E 01   -0.5015E 00
0.4723E 01   -0.4905E 00
0.4777E 01   -0.4792E 00
0.4830E 01   -0.4676E 00
0.4884E 01   -0.4557E 00
0.4938E 01   -0.4436E 00
0.4991E 01   -0.4313E 00
0.5045E 01   -0.4190E 00
0.5099E 01   -0.4066E 00
0.5152E 01   -0.3943E 00
0.5206E 01   -0.3820E 00
0.5260E 01   -0.3698E 00
0.5313E 01   -0.3577E 00
0.5367E 01   -0.3458E 00
0.5421E 01   -0.3341E 00
0.5474E 01   -0.3225E 00
0.5528E 01   -0.3112E 00
0.5582E 01   -0.3002E 00
0.5635E 01   -0.2893E 00
```

SECOND TEST RUN

```
SEARCH OF THE RADIUS

STARTING VALUES EB=  0.0        VO= 49.000000  RO=  7.000000  A=  0.520000

X1=  6.885442
 FINAL VALUES   EB=  0.0        VO= 49.000000  RO=  6.885501  A=  0.520000
```