Computational Physics Laboratory

(Coarse ID: PH573)

Assignment

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by

Mahasweta Pandit
Enrolment no. 414PH2049
National Institute of Technology , Rourkela
Department of Physics and Astronomy

I. INTRODUCTION

QUESTION: Study the solution of a Schrödinger equation for a system with neutron and proton(deuteron) moving in a simple box potential.

• A deuteron consists of a neutron and a proton.

• An interesting feature of Deuteron is that it does not have excited states because it is a weakly bound system.

• So, for a deuteron, only ground state of the system is studied.

• In analogy with the ground stat of the hydrogen atom, it is assumed that the ground state of the deuteron particle also has zero orbital angular momentum $\overrightarrow{L} = 0$

• As a simple model of this nucleus, one can consider a single particle of reduced mass μ is moving in a spherically-symmetric square potential well.

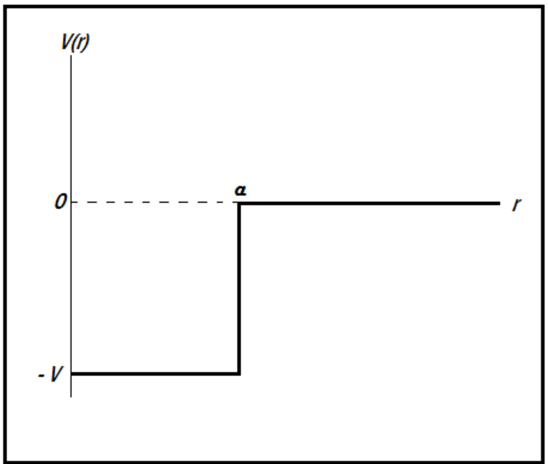
• Reduced mass μ:

$$\mu = \frac{m_p \times m_n}{m_p + m_n} \tag{1}$$

II. THREE DIMENSIONAL SPHERICALLY SYMMETRIC SQUARE-WELL POTENTIAL

The three dimensional spherically symmetric square-well potential can be expressed as,

$$\begin{aligned} V(r) &= -V_0 \quad at \quad 0 < r < a \\ &= 0 \qquad elsewhere \end{aligned} \tag{2}$$



Three-dimensional spherically symmetric square-well potential where, r represents the separation between the proton and neutron and a is nothing but the bond length or simply the diameter of the deuteron.

Total energy of a particle in the potential well is negative and its magnitude is less than the depth of the well. Since the potential is spherically symmetric, the Schrödinger equation can be solved by the technique of the separation of variables.

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi) \tag{3}$$

The solution of the angular part is nothing but the spherical harmonics$Y_{lm}(\theta,\phi)$ which can be found from the hydrogen problem. The radial part can be written as,

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR_l}{dr}) + [\frac{2\mu(V_0-|E|)}{\hbar^2} - \frac{l(l+1)}{r^2}]R_l = 0 \quad at \quad 0<r<a \tag{4}$$

and

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR_l}{dr}) - [\frac{2\mu|E|}{\hbar^2} + \frac{l(l+1)}{r^2}]R_l = 0 \quad elsewhere \tag{5}$$

Let us consider,

$$R_l = \frac{u(r)}{r} \tag{6}$$

and,

$$k_1^2 = \frac{2\mu|E|}{\hbar^2} \quad and \quad k_2^2 = \frac{2\mu(V_0-|E|)}{\hbar^2} \tag{7}$$

Then the radial equations will reduce to,

$$\frac{d^2u}{dr^2} + k_2^2u = 0 \quad at \quad 0<r<a \tag{8}$$

$$\frac{d^2u}{dr^2} - k_1^2u = 0 \quad elsewhere \tag{9}$$

and the solutions of these equations are,

$$u(r) = Asin(k_2r) + Bcos(k_2r) \quad at \quad 0<r<a \tag{10}$$

and

$$u(r) = Ce^{-k_1r} + De^{k_1r} \quad elsewhere \tag{11}$$

$u(r) \to 0$ as $r \to 0$, hence B is zero and also $u(r) \to 0$ as $r \to \infty$, hence D is also zero. Therefore the forms of solutions are,

$$u(r) = Asin(k_2r) \quad at \quad 0<r<a \tag{12}$$

and

$$u(r) = Ce^{-k_1 r} \quad elsewhere \tag{13}$$

Applying the Boundary condition that at $x = a$ $u(r)$ and its derivatives are continuous, one can get,

$$Asin(k_2 a) = Ce^{-k_1 a} \tag{14}$$

and

$$Ak_2 cos(k_2 a) = -Ck_1 e^{-k_1 a} \tag{15}$$

From the above two equations, one can get,

$$k_2 cot(k_2 a) = -k_1 \tag{16}$$

The above equation is a transcendental equation. By solving it graphically, one can calculate the binding energy of the deuteron. Also by using several methods like Bisection method, Newton-Raphson Method and Secant method.

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III. ALGORITHMS

A. Bisection Method

- **Step 1**: Read upper limit b and lower limit a
- **Step 2**: c = (a+b)/2
- **Step 3**: If $f(b) \times f(a) > 0$, the root is not in the interval given.
- **Step 4**: else if $f(a) == 0$, then root is a
- **Step 5**: else if $f(b) == 0$, then root is b
- **Step 6**: else if $f(c) == 0$, then root is c
- **Step 7**: else if $f(a) \times f(c) < 0$, then $b = c$
- **Step 8**: else if $f(b) \times f(c) < 0$, then $a = c$
- **Step 9**: else if abs$(b - a) > \epsilon$, then go to step 3
- **Step 10**: Solution is c.

B. Newton Raphson Method

- **Step 1**: Read trial solution E_n
- **Step 2**: If abs($f(x_n)/f'(x_n)) > \epsilon$ then
- **Step 3**: $x_{n1} = x_n - f(x_n)/f'(x_n)$

- **Step 4**: $x_n = x_{n+1}$
- **Step 5**: Go to step 2
- **Step 6**: Solution is x_{n+1}.

C. Secant Method

- **Step 1**: Read two approximate values a and b
- **Step 2**: If ((abs($a - b$) $> \epsilon$) or (abs($f(a) - f(b)$) $> \epsilon$)) then

$$\begin{aligned} e &= \frac{f(b) \times a - f(a) \times b}{f(b) - f(a)} \\ a &= b \\ b &= e \end{aligned}$$

- **Step 3**: Go to step 2
- **Step 4**: else stop. Solution is e

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IV. PROGRAM

```
PROGRAM boxpotential
IMPLICIT REAL (a-h,o-z)
!*****************************************************
!Mentioning the problem.
!*****************************************************
PRINT *,"The energy of a Deuteron in a box potential can be found
by solving a transcendental equation."
PRINT*,""
PRINT*,"The potential value has been considered to be 59.99 MeV
approximately."
PRINT*,""
PRINT*,"The equation can be solved using:"
PRINT*,"(1) Bisection Method;"
PRINT*,"(2) Newton-Raphson Method;"
PRINT*,"(3) Secant Method."
PRINT*,""
PRINT*,"Hit the  corresponding serial number for desired method."
READ*,j
!*****************************************************
!Calling the desired subroutine.
!******************************************************
IF(j==1)THEN
PRINT*,"Enter the approximate upper limit in MeV."
READ*,x
PRINT*,"Enter the approximate lower limit in MeV."
READ*,y
CALL bisect(x,y,bisec)
IF(bisec.GT. 0.0)THEN
PRINT*,"The Energy value found using Bisection Method is:",bisec,"MeV"
ELSE
PRINT*,""
```

```
PRINT*,"Please retry with another range."
END IF
ELSE IF (j==2)THEN
PRINT*,"Enter an approximate value of energy."
READ*,r
CALL newton(r,hnew)
IF(hnew.GT. 0.0)THEN
PRINT*,"The Energy value found using Newton-Raphson Method is:",hnew,"MeV"
ELSE
PRINT*,""
PRINT*,"Please retry with another range."
END IF
ELSE
PRINT*,"Enter one approximate value of E in MeV."
READ*,x
PRINT*,"Enter another approximate value of E in MeV."
READ*,y
CALL secant(x,y,sec)
IF(sec.GT. 0.0)THEN
PRINT*,"The Energy value found using Secand Method is:",sec,"MeV"
ELSE
PRINT*,""
PRINT*,"Please retry with another range."
END IF
END IF
END PROGRAM boxpotential
!*******************************************************
!Subroutine for Bisection method.
!*******************************************************
SUBROUTINE bisect(a,b,bisec)
fa = f(a)
fb = f(b)
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```
IF (fa*fb.GT.0) THEN
PRINT*,""
PRINT *,"Entries are invalid"
ELSE
PRINT*,""
PRINT*,"Starting iteration............"
PRINT*,""
do m= 1,30
xm = (b+a)/2
fxm = f(xm)
if(abs(fxm).lt. 0.00001) then
bisec = xm
return
else if ( sign(1.0,fa) == sign(1.0,fxm) ) then
a = xm
fa = fxm
else
b = xm
fb = fxm
end if
print *, m,")", xm,"MeV"
end do
end if
END SUBROUTINE bisect
!**********************************************************
!Subroutine for Newton-Raphson Method
!**********************************************************
SUBROUTINE newton(x,hnew)
INTEGER:: count
!REAL:: x,z,hnew
count=0
10 IF(df(x).EQ.0.0)THEN
```

```
PRINT*,"Incorrect trial."
STOP
ENDIF
z=x-(f(x)/df(x))
IF(abs(f(z)).LT.0.00001) GOTO 20
count=count+1
IF(count.GT.500)THEN
PRINT*,"An error has occured."
STOP
ENDIF
x=z
GOTO 10
20 hnew = x
RETURN
END SUBROUTINE newton
!***********************************************************
!Subroutine for Secant method.
!***********************************************************
SUBROUTINE secant(a,b,sec)
11  fa = f(a)
fb = f(b)
IF((abs(a-b).GT. 0.00001).OR.(abs(fa-fb).GT. 0.00001))THEN
s = (fb*a - fa*b)/(fb - fa)
a = b
b = s
GOTO 11
ELSE
sec = s
END IF
END SUBROUTINE secant
!***********************************************************
!Defining the function.
```

```
!**********************************************************
FUNCTION f(x)
REAL,INTENT(IN):: x
!PLANCK'S Constant : g(say) = h/(2*pi) = 6.582*(10**(-22)) MeV.s
!Reduced Mass : q = (mp*mn)/(mp + mn) = 5.216* (10**(-15))
!Bond Length : d = 1.25*(10**(-15)) m
! y= (sqrt(2q)*d)/g
y= 0.232
f = ((y*SQRT(60-x))/TAN(y*SQRT(60-x))) + (y*SQRT(x))
RETURN
END FUNCTION f
!**********************************************************
!Derivative of the function.
!**********************************************************
REAL FUNCTION df(x)
REAL,INTENT(IN):: x
y = 0.23277
t = y*SQRT(60 - x)
df =(y/2.0)*((y/((SIN(t))**2)) - (1/(SQRT(60-x)*TAN(t))) + (1/SQRT(x)))
RETURN
END FUNCTION df
```

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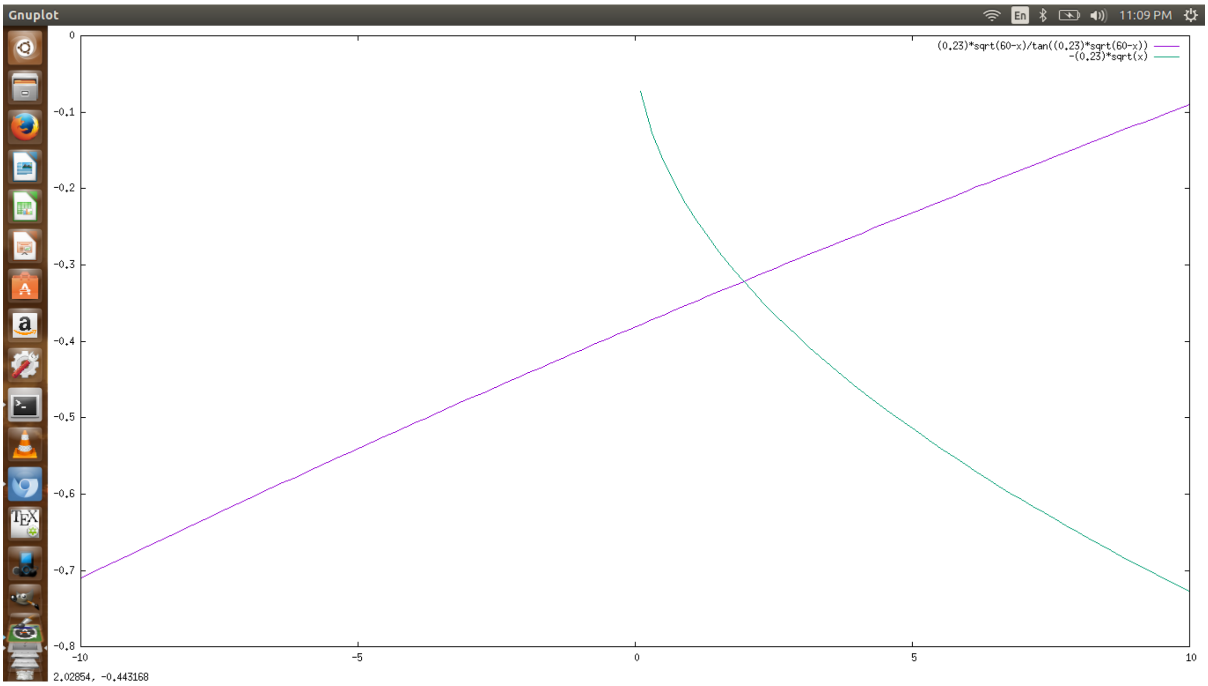
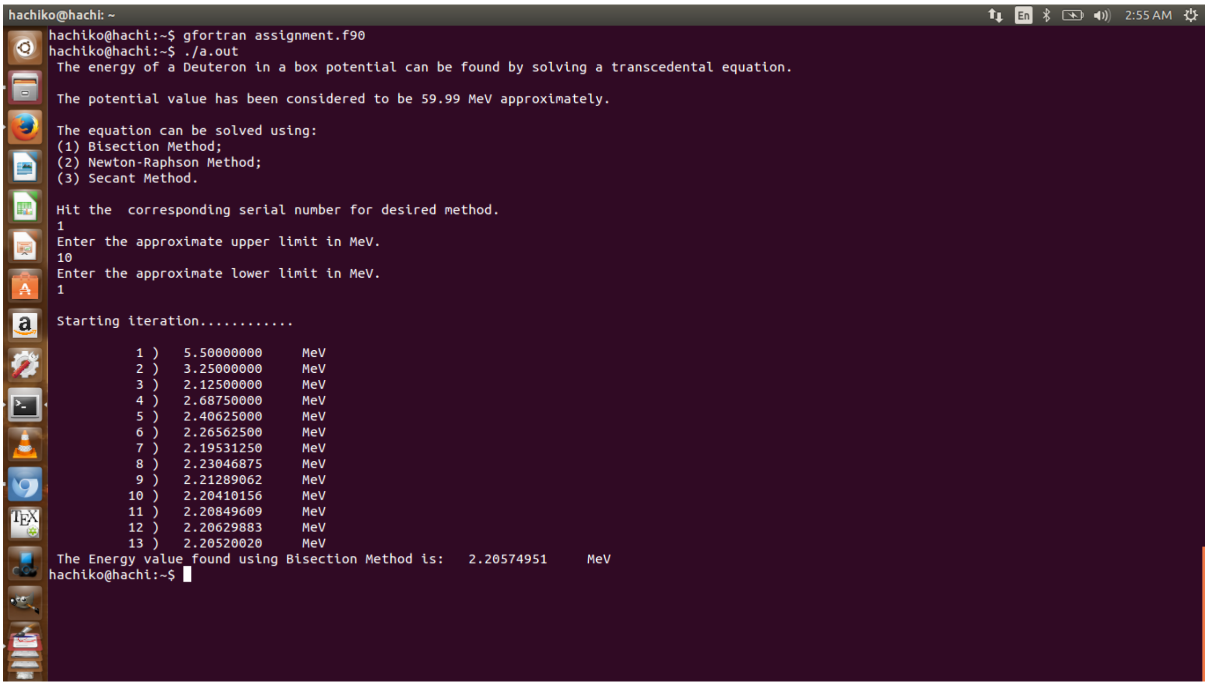
V. RESULTS

- The graphical solution using GNU plot:



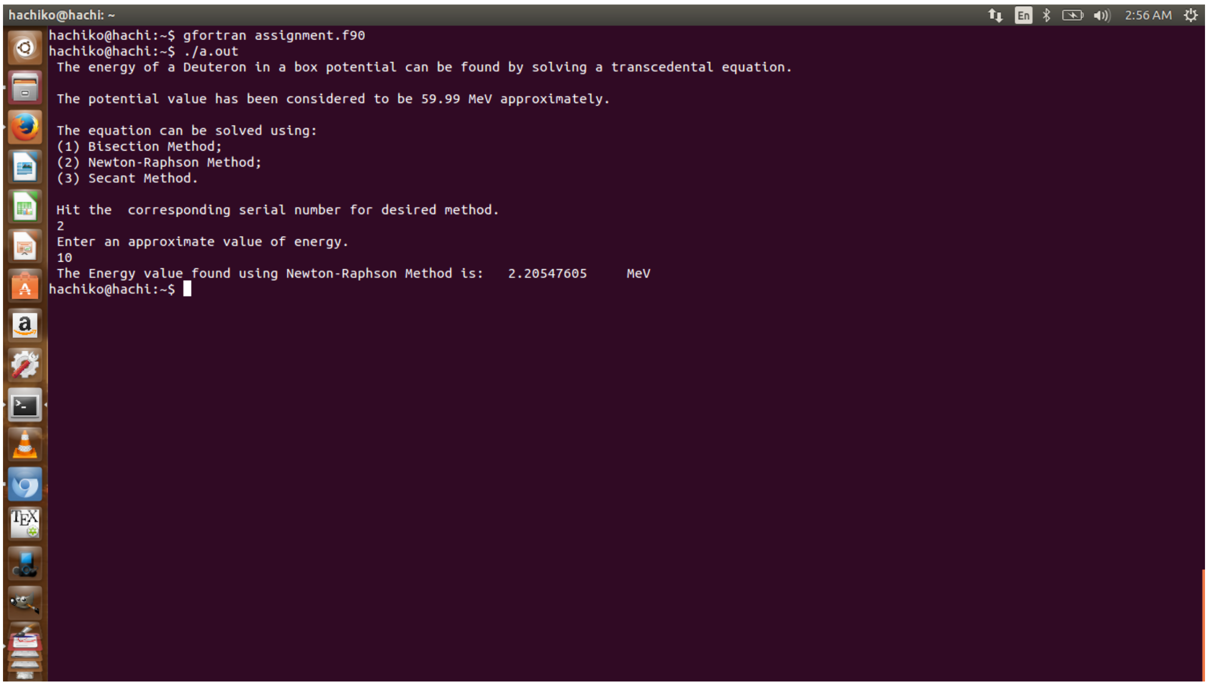
The binding energy found out: E = 2.223 MeV (approximately)

- Solution using Bisection method:



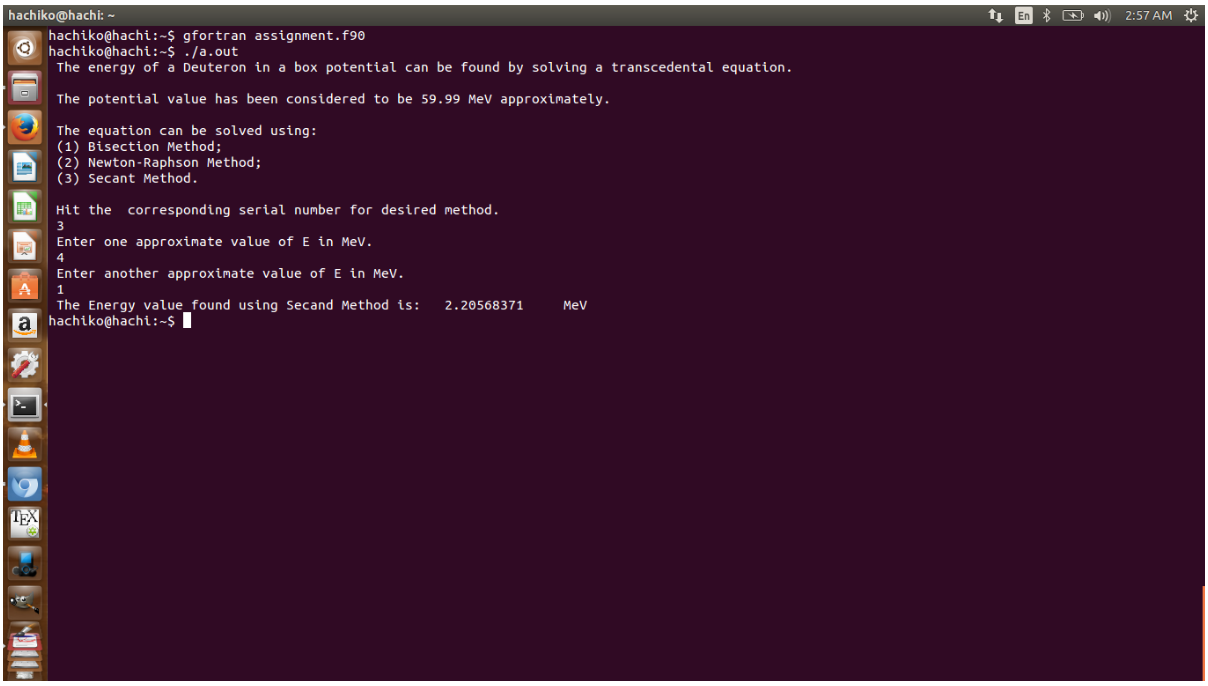
The binding energy found out: E = 2.20574951 MeV.

- Solution using Newton-Raphson Method:



The binding energy found out: E = 2.20547665 MeV.

- Solution using Secant Method:



The binding energy found out: E = 2.20568371 MeV.