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1 !PROGRAM 11 (OPTIONAL)
2 ! Name: Debasis Buxy
3 !PRN: 22020004154
4 !to find the first(even) eigen state of a particle in a FINITE WELL
5 module MODwell
6     implicit none
7     real, parameter :: TOL = 0.0001
8     real, parameter :: ZERO = 0.0000001
9     real, parameter :: MAXN = 50 !max number of iterations
10    real, parameter :: DEL = 0.1
11    real, parameter :: C1 = 1.88972599 !angstrom -> atomic unit
12    real, parameter :: C2 = 0.03674931 !eV -> hartree
13    real :: A, V0, lambda
14 end module MODwell
15
16 function FUNC(Z)
17     use MODwell
18     implicit none
19     real :: FUNC, Z
20     FUNC = (Z/cos(Z))*2 - lambda
21 end function FUNC
22
23 subroutine BOUNDS(B1,B2)
24     use MODwell
25     implicit none
26     real, intent(out) :: B1, B2
27     real :: FUNC,Z
28     Z = ZERO
29     do
30         if (FUNC(Z)*FUNC(Z+DEL) < 0.0) then
31             B1 = Z
32             B2 = Z+DEL
33             exit
34         end if
35         Z = Z+DEL
36     end do
37 end subroutine BOUNDS
38
39 function FINDROOT() !0 -> even, 1 -> odd
40     use MODwell
41     implicit none
42     real :: FINDROOT, FUNC, A1, A2, A3
43     integer :: N
44     N = 0
45     call BOUNDS(A1,A2)
46     do
47         N = N+1
48         A3 = (A1+A2)/2.0
49         if (N > MAXN) then
50             FINDROOT = A3
51             write(*,100) "Exceeded max iteration in interval", A1, A2
52             return
53         end if
54         if (abs(A1-A2) < TOL) then
55             FINDROOT = A3
56             write(*,100) "Root found in ",N," iterations"
57             return
58         end if
59         if (FUNC(A1)*FUNC(A3) < 0.0) then
60             A2 = A3

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61         else
62             A1 = A3
63         end if
64     end do
65 100 format(A,I0,A)
66 end function FINDROOT
67
68 function U1sq(X)
69     implicit none
70     real :: U1sq, X
71     U1sq = exp(2*X)
72 end function U1sq
73
74 function I1(D1,D2)
75     implicit none
76     real :: I1, U1sq, D1, D2
77     real :: H, S1, S2, S3
78     integer :: I,N
79     S1 = U1sq(D1)+U1sq(D2)
80     N = 100
81     H = (D2-D1)/N
82     S2 = 0.0
83     S3 = 0.0
84     do I = 1, N-1
85         if (mod(I,2) /= 0) then
86             S2 = S2 + U1sq(D1+I*H)
87         else
88             S3 = S3 + U1sq(D1+I*H)
89         end if
90     end do
91     I1 = (H/3.0)*(S1+4*S2+2*S3)
92 end function I1
93
94 function U2sq(X)
95     implicit none
96     real :: U2sq, X
97     U2sq = (cos(X))**2
98 end function U2sq
99
100 function I2(D1,D2)
101     implicit none
102     real :: I2, U2sq, D1, D2
103     real :: H, S1, S2, S3
104     integer :: I,N
105     S1 = U2sq(D1)+U2sq(D2)
106     N = 100
107     H = (D2-D1)/N
108     S2 = 0.0
109     S3 = 0.0
110     do I = 1, N-1
111         if (mod(I,2) /= 0) then
112             S2 = S2 + U2sq(D1+I*H)
113         else
114             S3 = S3 + U2sq(D1+I*H)
115         end if
116     end do
117     I2 = (H/3.0)*(S1+4*S2+2*S3)
118 end function I2
119
120 function U3sq(X)

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121     implicit none
122     real :: U3sq, X
123     U3sq = exp(-2*X)
124 end function U3sq
125
126 function I3(D1,D2)
127     implicit none
128     real :: I3, U3sq, D1, D2
129     real :: H, S1, S2, S3
130     integer :: I,N
131     S1 = U3sq(D1)+U3sq(D2)
132     N = 100
133     H = (D2-D1)/N
134     S2 = 0.0
135     S3 = 0.0
136     do I = 1, N-1
137         if (mod(I,2) /= 0) then
138             S2 = S2 + U3sq(D1+I*H)
139         else
140             S3 = S3 + U3sq(D1+I*H)
141         end if
142     end do
143     I3 = (H/3.0)*(S1+4*S2+2*S3)
144 end function I3
145
146 program FINITEWELL
147     use MODwell
148     implicit none
149     real :: FINDROOT, FUNC, X0, Y0, I1, I2, I3
150     real :: ENERGY, CbyD, L1, L2, C, D, X ,delX
151     real :: ALPHA, BETA ! alpha, q
152     real :: P, Q, R, Itotal
153     real :: WIDTH = 1 !in angstrom
154     real :: HEIGHT = 5 !in eV
155
156     open(unit=1, file="wellout1.txt")
157     open(unit=2, file="wellout2.txt")
158     open(unit=3, file="wellout3.txt")
159
160     A = WIDTH*C1 !in au
161     V0 = HEIGHT*C2 !in hartree
162     lambda = 2*A**2*V0 !lambda = Z0**2, Z0 = sqrt(2mV0)*(A/h')**2, m->1, h'->1
163     Y0 = FINDROOT()
164     X0 = Y0*tan(Y0)
165     ALPHA = X0/A
166     BETA = Y0/A
167     ENERGY = 0.5*(2*V0 - (BETA)**2)/C2
168     CbyD = cos(Y0)*exp(X0)
169     L1 = ALPHA*A
170     L2 = BETA*A
171     P = I1(-5*L1, -1*L1)
172     Q = I2(-L2,L2)
173     R = I3(L1, 5*L1)
174     Itotal = ((CbyD**2/ALPHA)*(P+R))+(Q/BETA)
175     D = 1.0/sqrt(Itotal)
176     C = CbyD*D
177     delX = 0.01
178     X = -10*A
179     do
180         if (X > -1*A) exit

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181         write(1,*) X, (C*exp(ALPHA*X))**2
182         X = X+delX
183     end do
184     do
185         if (X > A) exit
186         write(2,*) X, (D*cos(BETA*X))**2
187         X = X+delX
188     end do
189     do
190         if (X > 10*A) exit
191         write(3,*) X, (C*exp(-1*ALPHA*X))**2
192         X = X+delX
193     end do
194
195     write(*,110) "a(angstrom)", WIDTH
196     write(*,110) "V0(eV)", HEIGHT
197     write(*,110) "a(au)", A
198     write(*,110) "V0(hartree)", V0
199     write(*,110) "lambda", lambda
200     write(*,110) "Root", Y0
201     write(*,110) "F(root)", FUNC(Y0)
202     write(*,110) "Energy(eV)", ENERGY
203     write(*,110) "q**2+a**2", (BETA**2+ALPHA**2)
204     write(*,110) "2*V0", 2*V0
205     write(*,110) "C/A", CbyD
206     write(*,110) "C", C
207     write(*,110) "A", D
208     write(*,110) "alpha", ALPHA
209     write(*,110) "q", BETA
210 110 format(A,T16,': ',F10.6)
211 end program FINITEWELL

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