HW3 Solutions
Computational Physics
Spring 2004

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schdebug

Here we test the function schint:

```
E=-.5
============================================================
Outward integration test:
-------------------------
   0 nodes
   Return value of Psi: 24430075685.431213378906

   k           r             Psianal          Psiout       Psiout/Psianal
   0   0.000000000000   0.000000000000   0.000000000000              nan
   2   0.000408163265   0.000407996702   0.000407939039   0.999858668393
   4   0.001666666667   0.001663891202   0.001663809564   0.999950935283
   6   0.003829787234   0.003815148014   0.003815047596   0.999973679188
   8   0.006956521739   0.006908296479   0.006908178397   0.999982907289
  10   0.011111111111   0.010988337659   0.010988201652   0.999987622613
  12   0.016363636364   0.016098046701   0.016097891867   0.999990381826
  14   0.022790697674   0.022277155989   0.022276981074   0.999992148236
  16   0.030476190476   0.029561402717   0.029561206253   0.999993354045
  18   0.039512195122   0.037981422796   0.037981203183   0.999994217894
  20   0.050000000000   0.047561471225   0.047561226787   0.999994860579
  22   0.062051282051   0.058317947363   0.058317676390   0.999995353532
  24   0.075789473684   0.070257702035   0.070257402833   0.999995741351
  26   0.091351351351   0.083376102245   0.083375773173   0.999996053160
  28   0.108888888889   0.097654828728   0.097654468258   0.999996308738
  30   0.128571428571   0.113059382067   0.113058988845   0.999996521994
  32   0.150588235294   0.129536275049   0.129535847975   0.999996703051
  34   0.175151515152   0.147009893179   0.147009431501   0.999996859549
  36   0.202500000000   0.165379012726   0.165378516174   0.999996997492
```

```
  38   0.232903225806   0.184512977839   0.184512446781   0.999997121843
  40   0.266666666667   0.204247556897   0.204246992551   0.999997236952
  42   0.304137931034   0.224380526141   0.224379930841   0.999997346919
  44   0.345714285714   0.244667069005   0.244666446551   0.999997455913
  46   0.391851851852   0.264815137326   0.264814493430   0.999997568507
  48   0.443076923077   0.284481001606   0.284480344474   0.999997690064
  50   0.500000000000   0.303265329856   0.303264670927   0.999997827217
  52   0.563333333333   0.320710287970   0.320709642865   0.999997988512
  54   0.633913043478   0.336298361352   0.336297751069   0.999998185294
  56   0.712727272727   0.349453871192   0.349453323585   0.999998432964
  58   0.800952380952   0.359548513373   0.359548064942   0.999998752795
  60   0.900000000000   0.365912693767   0.365912391744   0.999999174605
  62   1.011578947368   0.367854969544   0.367854874171   0.999999740733
  64   1.137777777778   0.364692503911   0.364692690679   1.000000512124
  66   1.281176470588   0.355796017414   0.355796578825   1.000001577900
  68   1.445000000000   0.340653080623   0.340654126854   1.000003071251
  70   1.633333333333   0.318953352632   0.318955010639   1.000005198277
  72   1.851428571429   0.290697802856   0.290700215066   1.000008297997
  74   2.106153846154   0.256329799646   0.256333129787   1.000012991625
  76   2.406666666667   0.216877196055   0.216881670259   1.000020630126
  78   2.765454545455   0.174078395667   0.174084466926   1.000034876578
  80   3.200000000000   0.130439052731   0.130447941683   1.000068146402
  82   3.735555555556   0.089130026376   0.089145322491   1.000171615737
  84   4.410000000000   0.053604336435   0.053636410142   1.000598341646
  86   5.282857142857   0.026825829563   0.026903301225   1.002887950302
  88   6.453333333333   0.010165694209   0.010364660709   1.019572347466
  90   8.100000000000   0.002458667018   0.002999763955   1.220077356077
  92  10.580000000000   0.000268936686   0.002476428839   9.208222479310
  94  14.726666666667   0.000005920991   0.043930704858 7419.485404315251
  96  23.040000000000   0.000000002272  10.755736007182 4734809632.776056289673
  98  48.020000000000   0.000000000000 144871.469697265828 215964183274403735273472O.00000
 100              inf              nan 24430075685.431213378906              nan
============================================================
Inward integration test:
------------------------
   0 nodes
   Return value of Psi: 2.443007568612e+10

   k           r             Psianal          Psiout       Psiout/Psianal
   0   0.000000000000   0.000000000000 2.443007568612e+10              inf
   2   0.000408163265   0.000407996702 1.367428822364e+13 3.351568322720e+16
   4   0.001666666667   0.001663891202 5.569625775551e+13 3.347349735041e+16
   6   0.003829787234   0.003815148014 1.276775018934e+14 3.346593668641e+16
   8   0.006956521739   0.006908296479 2.311747312891e+14 3.346334830791e+16
  10   0.011111111111   0.010988337659 3.676936177715e+14 3.346216954630e+16
  12   0.016363636364   0.016098046701 5.386653813620e+14 3.346153675397e+16
```

14	0.022790697674	0.022277155989	7.454194414504e+14	3.346115822967e+16
16	0.030476190476	0.029561402717	9.891515426606e+14	3.346091361576e+16
18	0.039512195122	0.037981422796	1.270886742147e+15	3.346074603293e+16
20	0.050000000000	0.047561471225	1.591436591711e+15	3.346062581163e+16
22	0.062051282051	0.058317947363	1.951349792630e+15	3.346053626495e+16
24	0.075789473684	0.070257702035	2.350855550841e+15	3.346046743252e+16
26	0.091351351351	0.083376102245	2.789798821724e+15	3.346041307516e+16
28	0.108888888889	0.097654828728	3.267566616134e+15	3.346036912559e+16
30	0.128571428571	0.113059382067	3.783004554861e+15	3.346033284200e+16
32	0.150588235294	0.129536275049	4.334322924944e+15	3.346030232305e+16
34	0.175151515152	0.147009893179	4.918991632589e+15	3.346027621838e+16
36	0.202500000000	0.165379012726	5.533623697644e+15	3.346025354987e+16
38	0.232903225806	0.184512977839	6.173847340401e+15	3.346023359832e+16
40	0.266666666667	0.204247556897	6.834167336527e+15	3.346021582998e+16
42	0.304137931034	0.224380526141	7.507817246789e+15	3.346019984850e+16
44	0.345714285714	0.244667069005	8.186605481321e+15	3.346018536374e+16
46	0.391851851852	0.264815137326	8.860760088737e+15	3.346017217226e+16
48	0.443076923077	0.284481001606	9.518779872473e+15	3.346016014681e+16
50	0.500000000000	0.303265329856	1.014730319426e+16	3.346014923323e+16
52	0.563333333333	0.320710287970	1.073101095998e+16	3.346013945454e+16
54	0.633913043478	0.336298361352	1.125258720000e+16	3.346013092296e+16
56	0.712727272727	0.349453871192	1.169276981395e+16	3.346012386144e+16
58	0.800952380952	0.359548513373	1.203053591365e+16	3.346011863824e+16
60	0.900000000000	0.365912693767	1.224348111336e+16	3.346011581980e+16
62	1.011578947368	0.367854969544	1.230847004455e+16	3.346011625127e+16
64	1.137777777778	0.364692503911	1.220265537504e+16	3.346012118203e+16
66	1.281176470588	0.355796017414	1.190498187533e+16	3.346013247098e+16
68	1.445000000000	0.340653080623	1.139830418130e+16	3.346015295221e+16
70	1.633333333333	0.318953352632	1.067223887725e+16	3.346018716905e+16
72	1.851428571429	0.290697802856	9.726819142341e+15	3.346024306606e+16
74	2.106153846154	0.256329799646	8.576881335257e+15	3.346033643804e+16
76	2.406666666667	0.216877196055	7.256820280023e+15	3.346050397194e+16
78	2.765454545455	0.174078395667	5.824810202927e+15	3.346084492906e+16
80	3.200000000000	0.130439052731	4.364707826017e+15	3.346166454479e+16
82	3.735555555556	0.089130026376	2.982647518833e+15	3.346400354744e+16
84	4.410000000000	0.053604336435	1.794230721699e+15	3.347174577709e+16
86	5.282857142857	0.026825829563	8.986852474240e+14	3.350074394971e+16
88	6.453333333333	0.010165694209	3.417964463181e+14	3.362253863631e+16
90	8.100000000000	0.002458667018	8.411510813461e+13	3.421167140723e+16
92	10.580000000000	0.000268936686	1.020023736853e+13	3.792802504888e+16
94	14.726666666667	0.000005920991	3.982693370521e+11	6.726396817028e+16
96	23.040000000000	0.000000002272	1.950227108993e+09	8.585143867044e+17
98	48.020000000000	0.000000000000	1.633746550000e+05	2.435474286866e+24
100	inf	nan	0.000000000000e+00	nan

Notice that on the inward integration, we don't quite reach zero; we expect this to improve for greater N.

A test of node counting just above the second exited state:

```
E=-.05
============================================================
Outward integration test:
-------------------------
   3 nodes
.
.
.
============================================================
Inward integration test:
-------------------------
   3 nodes
.
.
.
```

Edebug

Searching for the ground state:

```
E1=-1.0
E2=-.3
Search for energy in range ( -1.0000000000000000, -0.3000000000000000):
N=10
   (50 iterations in rtbisp480, func=1.236754e-13)
Solution from rtbisp480:  E= -0.4854389178271255
   (8 iterations in zriddrp480, fnew=1.581913e-14)
Solution from zriddrp480: E= -0.4854389178271258
Search for energy in range ( -1.0000000000000000, -0.3000000000000000):
N=100
   (50 iterations in rtbisp480, func=4.998395e+00)
Solution from rtbisp480:  E= -0.4999985397456193
   (6 iterations in zriddrp480, fnew=-5.013834e-01)
Solution from zriddrp480: E= -0.4999985397456195
Search for energy in range ( -1.0000000000000000, -0.3000000000000000):
N=1000
   (50 iterations in rtbisp480, func=8.859815e+47)
Solution from rtbisp480:  E= -0.4999999998459483
   (13 iterations in zriddrp480, fnew=7.326148e+46)
Solution from zriddrp480: E= -0.4999999998459486
Search for energy in range ( -1.0000000000000000, -0.3000000000000000):
N=10000
   (50 iterations in rtbisp480, func=-1.080807e-102)
Solution from rtbisp480:  E= -0.4999999999999837
   (10 iterations in zriddrp480, fnew=-2.095120e-101)
Solution from zriddrp480: E= -0.4999999999999836
Search for energy in range ( -1.0000000000000000, -0.3000000000000000):
N=100000
   (50 iterations in rtbisp480, func=-1.507457e+85)
Solution from rtbisp480:  E= -0.5000000000000024
   (13 iterations in zriddrp480, fnew=3.424516e+84)
Solution from zriddrp480: E= -0.5000000000000030
```

Searching for the first excited state:

```
E1=-.2
E2=-.1
Search for energy in range ( -0.2000000000000000, -0.1000000000000000):
N=1000
   (47 iterations in rtbisp480, func=-1.916153e+27)
Solution from rtbisp480:  E= -0.1249999989678650
   (7 iterations in zriddrp480, fnew=-2.204524e+25)
Solution from zriddrp480: E= -0.1249999989678645
```

```
Search for energy in range ( -0.2000000000000000, -0.1000000000000000):
N=10000
   (47 iterations in rtbisp480, func=9.209434e+133)
Solution from rtbisp480:  E= -0.1249999999998977
   (8 iterations in zriddrp480, fnew=5.570422e+132)
Solution from zriddrp480: E= -0.1249999999998974
```

Second excited state:

```
E1=-.1
E2=-.05
Search for energy in range ( -0.1000000000000000, -0.0500000000000000):
N=1000
   (46 iterations in rtbisp480, func=-8.138717e+17)
Solution from rtbisp480:  E= -0.0555555382690919
   (8 iterations in zriddrp480, fnew=1.236101e+16)
Solution from zriddrp480: E= -0.0555555382690926
Search for energy in range ( -0.1000000000000000, -0.0500000000000000):
N=10000
   (46 iterations in rtbisp480, func=-3.419517e+103)
Solution from rtbisp480:  E= -0.0555555555538426
   (8 iterations in zriddrp480, fnew=-1.287723e+102)
Solution from zriddrp480: E= -0.0555555555538427
```

How many more can we get?

Note that Ridder's method is spectacularly better than bisection; see NR for a precise notion of 'better'.