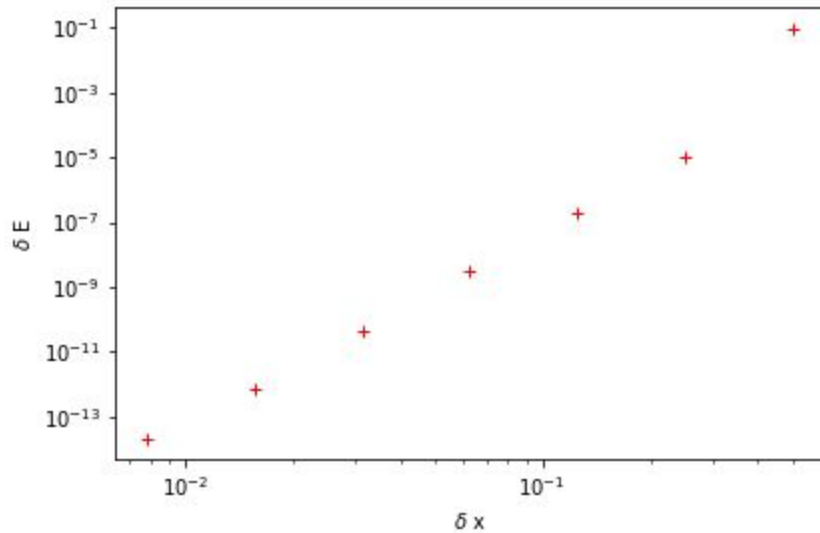


Rachel Buttry
PHYS 305
Homework #6

Problem 1

a)



slope = 5.83973194723

1.35308431126e-16 [1. 1.5]

y - y0 = [-2.47135645282e-13 -1.487698853e-13]

It's time reversible

b) For $|E - E_0| < 10^{-4}$, eta = 0.1

Output:

Command-line parameters:

```
{'N': 50,  
'dt_dia': 0.5,  
'dt_param': 0.1,  
'eps': 0.001,  
'fixed_dt': False,  
'seed': 12345,  
't_end': 20.0,  
'v0': 0.7}
```

t = 0.499, dE = -1.410e-09, ddE = -1.410e-09, steps = 133

t = 0.999, dE = -5.175e-09, ddE = -3.764e-09, steps = 280

t = 1.499, dE = -1.070e-08, ddE = -5.530e-09, steps = 514

t = 2.000, dE = -1.163e-08, ddE = -9.260e-10, steps = 701

t = 2.501, dE = -1.687e-08, ddE = -5.244e-09, steps = 959
 t = 3.001, dE = -2.533e-08, ddE = -8.458e-09, steps = 1244
 t = 3.500, dE = -3.423e-08, ddE = -8.896e-09, steps = 1517
 t = 4.000, dE = -4.154e-08, ddE = -7.307e-09, steps = 1843
 t = 4.500, dE = -4.535e-08, ddE = -3.810e-09, steps = 2061
 t = 5.000, dE = -4.886e-08, ddE = -3.510e-09, steps = 2280
 t = 5.499, dE = -6.417e-08, ddE = -1.532e-08, steps = 2580
 t = 6.000, dE = -7.425e-08, ddE = -1.008e-08, steps = 2801
 t = 6.500, dE = -7.694e-08, ddE = -2.681e-09, steps = 2999
 t = 6.999, dE = -7.772e-08, ddE = -7.819e-10, steps = 3130
 t = 7.499, dE = -8.242e-08, ddE = -4.705e-09, steps = 3364
 t = 7.998, dE = -9.432e-08, ddE = -1.190e-08, steps = 3576
 t = 8.500, dE = -1.063e-07, ddE = -1.196e-08, steps = 3844
 t = 8.998, dE = -1.080e-07, ddE = -1.744e-09, steps = 4014
 t = 9.500, dE = -1.239e-07, ddE = -1.583e-08, steps = 4421
 t = 10.001, dE = -1.365e-07, ddE = -1.260e-08, steps = 4795
 t = 10.500, dE = -1.847e-07, ddE = -4.825e-08, steps = 5331
 t = 11.000, dE = -2.511e-07, ddE = -6.638e-08, steps = 5974
 t = 11.500, dE = -2.683e-07, ddE = -1.726e-08, steps = 6470
 t = 12.002, dE = -2.914e-07, ddE = -2.310e-08, steps = 7009
 t = 12.500, dE = -4.177e-07, ddE = -1.263e-07, steps = 8249
 t = 13.000, dE = -5.415e-07, ddE = -1.238e-07, steps = 9351
 t = 13.500, dE = -6.104e-07, ddE = -6.892e-08, steps = 10978
 t = 14.000, dE = -7.184e-07, ddE = -1.080e-07, steps = 12924
 t = 14.500, dE = -8.445e-07, ddE = -1.261e-07, steps = 14908
 t = 15.000, dE = -9.516e-07, ddE = -1.071e-07, steps = 16824
 t = 15.500, dE = -1.089e-06, ddE = -1.376e-07, steps = 18497
 t = 16.000, dE = -1.118e-06, ddE = -2.898e-08, steps = 19291
 t = 16.501, dE = -1.139e-06, ddE = -2.039e-08, steps = 19841
 t = 17.000, dE = -1.158e-06, ddE = -1.902e-08, steps = 20457
 t = 17.500, dE = -1.174e-06, ddE = -1.600e-08, steps = 21399
 t = 18.000, dE = -1.326e-06, ddE = -1.527e-07, steps = 23522
 t = 18.500, dE = -1.477e-06, ddE = -1.509e-07, steps = 25411
 t = 19.000, dE = -1.552e-06, ddE = -7.453e-08, steps = 26668
 t = 19.500, dE = -1.622e-06, ddE = -7.068e-08, steps = 28242
 t = 20.000, dE = -1.633e-06, ddE = -1.098e-08, steps = 31034

c) Kinetic energy stabilizes at t = 4.93049352242

Output:

Command-line parameters:

```

{'N': 50,
'dt_dia': 0.5,
'dt_param': 0.1,

```

'eps': 0.001,
'fixed_dt': False,
'seed': 12345,
't_end': 20.0,
'v0': 0.7}

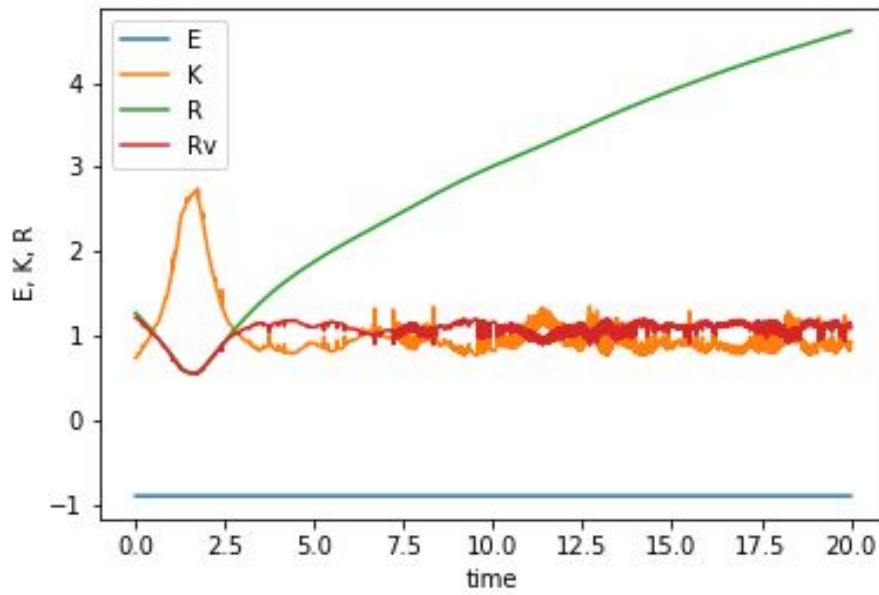
t = 0.501, dE = -2.704e-09, ddE = -2.704e-09, steps = 140
t = 1.000, dE = -5.673e-09, ddE = -2.969e-09, steps = 315
t = 1.501, dE = -1.163e-08, ddE = -5.959e-09, steps = 659
t = 2.001, dE = -1.249e-08, ddE = -8.628e-10, steps = 1003
t = 2.500, dE = -2.017e-08, ddE = -7.680e-09, steps = 1274
t = 3.000, dE = -2.220e-08, ddE = -2.022e-09, steps = 1426
t = 3.499, dE = -2.416e-08, ddE = -1.966e-09, steps = 1601
t = 4.000, dE = -3.039e-08, ddE = -6.229e-09, steps = 1855
t = 4.501, dE = -3.117e-08, ddE = -7.789e-10, steps = 2050

Kinetic energy slope = 7.65228369045e-05 , t = 4.93049352242

t = 4.999, dE = -3.122e-08, ddE = -5.202e-11, steps = 2215
t = 5.500, dE = -3.898e-08, ddE = -7.763e-09, steps = 2494
t = 5.998, dE = -4.285e-08, ddE = -3.869e-09, steps = 2744
t = 6.499, dE = -4.607e-08, ddE = -3.215e-09, steps = 2982
t = 7.000, dE = -5.871e-08, ddE = -1.264e-08, steps = 3317
t = 7.500, dE = -9.908e-08, ddE = -4.037e-08, steps = 3839
t = 8.000, dE = -1.903e-07, ddE = -9.124e-08, steps = 4937
t = 8.500, dE = -2.869e-07, ddE = -9.659e-08, steps = 6287
t = 8.999, dE = -2.939e-07, ddE = -7.014e-09, steps = 6805
t = 9.500, dE = -3.036e-07, ddE = -9.632e-09, steps = 7326
t = 10.000, dE = -3.937e-07, ddE = -9.011e-08, steps = 8126
t = 10.500, dE = -4.503e-07, ddE = -5.669e-08, steps = 9208
t = 11.000, dE = -5.500e-07, ddE = -9.966e-08, steps = 10471
t = 11.499, dE = -6.735e-07, ddE = -1.235e-07, steps = 11699
t = 12.000, dE = -8.646e-07, ddE = -1.910e-07, steps = 12945
t = 12.500, dE = -1.050e-06, ddE = -1.850e-07, steps = 14274
t = 13.000, dE = -1.268e-06, ddE = -2.186e-07, steps = 15887
t = 13.500, dE = -1.514e-06, ddE = -2.463e-07, steps = 17636
t = 14.000, dE = -1.764e-06, ddE = -2.491e-07, steps = 19152
t = 14.500, dE = -1.803e-06, ddE = -3.980e-08, steps = 20159
t = 15.000, dE = -1.821e-06, ddE = -1.731e-08, steps = 21079
t = 15.500, dE = -1.848e-06, ddE = -2.724e-08, steps = 22056
t = 16.000, dE = -1.873e-06, ddE = -2.518e-08, steps = 23053
t = 16.500, dE = -1.890e-06, ddE = -1.736e-08, steps = 23962
t = 17.001, dE = -1.914e-06, ddE = -2.389e-08, steps = 24849
t = 17.500, dE = -1.993e-06, ddE = -7.885e-08, steps = 25898
t = 18.000, dE = -2.129e-06, ddE = -1.363e-07, steps = 26950
t = 18.500, dE = -2.335e-06, ddE = -2.054e-07, steps = 28245

t = 19.000, dE = -2.410e-06, ddE = -7.496e-08, steps = 29076
t = 19.500, dE = -2.466e-06, ddE = -5.647e-08, steps = 30111
t = 20.000, dE = -2.545e-06, ddE = -7.897e-08, steps = 31142

Plot:



Problem 2

Deviation from Runge-Kutta 6 $dx = 0.001$

	Midpoint	RK4	RK6
dx = 0.1	nan	5.49023801e-02	6.65237138e-04
dx = 0.01	7.08677161e-01	9.75840035e-05	1.15720251e-08
dx = 0.001	8.31652530e-02	4.50211311e-07	0.00000000e+00

Output:

$z = \text{nan}$ $g(z) = \text{nan}$

$z = 66.3653015877$ $g(z) = -9.65894031424\text{e-}15$

$z = 66.4268197206$ $g(z) = -1.15463194561\text{e-}14$

$z = 64.5565266195$ $g(z) = -1.02140518266\text{e-}14$

$z = 66.4255989136$ $g(z) = 8.43769498715\text{e-}15$

$z = 66.425644948$ $g(z) = -1.11022302463\text{e-}16$

$z = 65.6389694214$ $g(z) = 5.3290705182\text{e-}15$

$z = 66.4256377764$ $g(z) = -1.22124532709\text{e-}15$

$z = 66.4256449853$ $g(z) = 2.59792187762\text{e-}14$

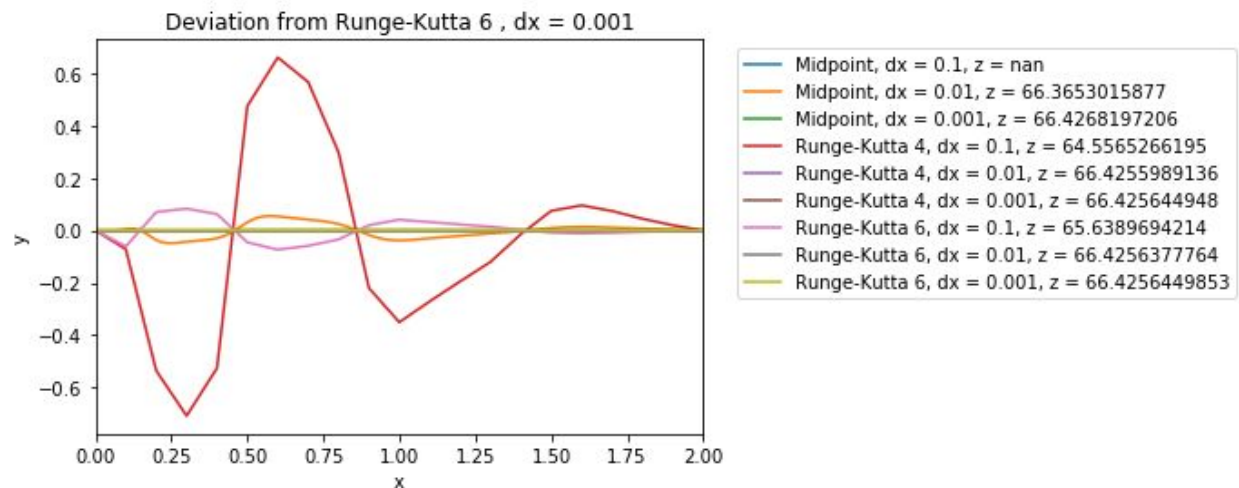
Maximum Absolute Difference

[nan 5.49023801e-02 6.65237138e-04]

[7.08677161e-01 9.75840035e-05 1.15720251e-08]

[8.31652530e-02 4.50211311e-07 0.00000000e+00]

Plot:



The decrease in order of integration methods created more "error" than the increase in dx .

Problem 3

a) Proof:

$$\frac{1}{r^2} (r^2 R')' + \left[\frac{2m_e}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} + E \right) - \frac{l(l+1)}{r^2} \right] R = 0$$

$$R' = \frac{dR}{dr} \quad a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} \quad E_0 = m_e c^2 / (32\pi^2 \epsilon_0^2 \hbar^2)$$

$$u = du/dx \quad z = E/E_0 \quad \chi = r/a_0 \quad \frac{dr}{dx} = a_0; \quad \frac{dR}{dx} = \frac{dR}{dr} \frac{dr}{dx}$$

$$\frac{2m_e}{\hbar^2} a_0^2 = \frac{16\pi^2 \epsilon_0^2 \hbar^4}{m_e^2 e^4} \cdot \frac{2m_e}{\hbar^2} = \frac{32\pi^2 \epsilon_0^2 \hbar^2}{m_e e^4} = \frac{1}{E_0}$$

$$\left[\frac{m_e e^2}{4\pi\epsilon_0 \hbar^2} \frac{1}{r} + \frac{2m_e}{\hbar^2} E - \frac{l(l+1)}{r^2} \right] R = \frac{a_0^2}{d_0^2} R$$

$$= \left[\frac{z}{a_0 r} a_0^2 + \frac{2m_e}{\hbar^2} a_0^2 E - \frac{l(l+1)}{r^2} \right] \frac{R}{d_0^2} = \left[\frac{z}{\chi} + z - \frac{l(l+1)}{\chi^2} \right] \frac{R}{a_0^2}$$

$$\frac{1}{r^2} (r^2 R')' + \left[z + \frac{z}{\chi} - \frac{l(l+1)}{\chi^2} \right] \frac{R}{a_0^2} = 0$$

$$\frac{a_0}{r} (r^2 R')' + \left[z + \frac{z}{\chi} - \frac{l(l+1)}{\chi^2} \right] \frac{1}{a_0} R = 0$$

$$\frac{1}{\chi} (r^2 R')' + \left[z + \frac{z}{\chi} - \frac{l(l+1)}{\chi^2} \right] u = 0$$

$$\frac{1}{\chi} (r^2 \frac{dR}{dr})' = \frac{a_0}{r} \left[2r \frac{dR}{dr} + r^2 \frac{d^2 R}{dr^2} \right] = a_0 \left[2 \frac{dR}{dr} + r \frac{d^2 R}{dr^2} \right]$$

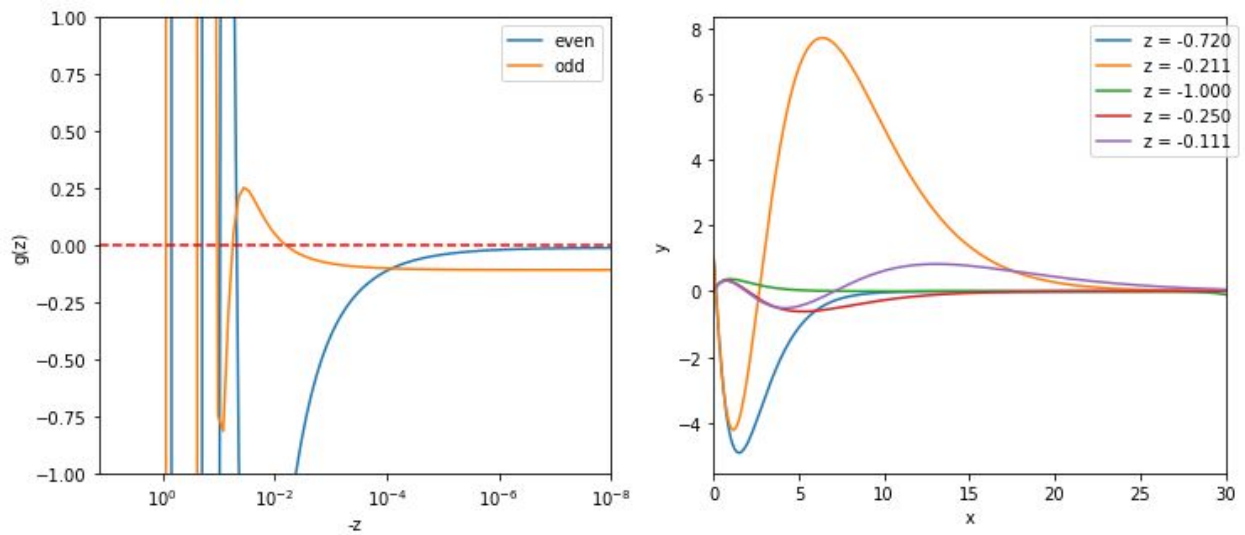
$$u' = \frac{d}{dx} (x R) = R + x \frac{dR}{dx} = R + a_0 x \frac{dR}{dr}$$

$$u'' = \frac{d^2}{dx^2} (x R) = \frac{dR}{dx} + \left[a_0 \frac{dR}{dr} + a_0 x \frac{d}{dx} \left(\frac{dR}{dr} \right) \right] = 2a_0 \frac{dR}{dr} + \frac{a_0 r}{a_0} \frac{d}{dr} \left(\frac{dR}{dr} \right) =$$

$$= 2a_0 \frac{dR}{dr} + r \frac{d}{dr} (a_0 \frac{dR}{dr}) = a_0 \left[2 \frac{dR}{dr} + r \frac{d^2 R}{dr^2} \right]$$

$$u'' + \left[z + \frac{z}{\chi} - \frac{l(l+1)}{\chi^2} \right] u = 0$$

b)



Only plotted the first 5, but found the following solutions:

Even

$$z = -0.720104488233 \quad g(z) = 0.0177187316713$$

$$z = -0.210503587396 \quad g(z) = -1.97059480279e-10$$

$$z = -0.0987171355425 \quad g(z) = 3.3003116906e-09$$

$$z = -0.0483479716389 \quad g(z) = -3.87361254184e-10$$

Odd

$$z = -0.999999999422 \quad g(z) = -0.20392069564$$

$$z = -0.249999999381 \quad g(z) = 9.56443454312e-08$$

$$z = -0.111055560996 \quad g(z) = -4.82997624535e-10$$

$$z = -0.0568822774509 \quad g(z) = 7.30828869644e-11$$

$$z = -0.0063016561319 \quad g(z) = 7.36424810022e-12$$