Homework 1

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06-640

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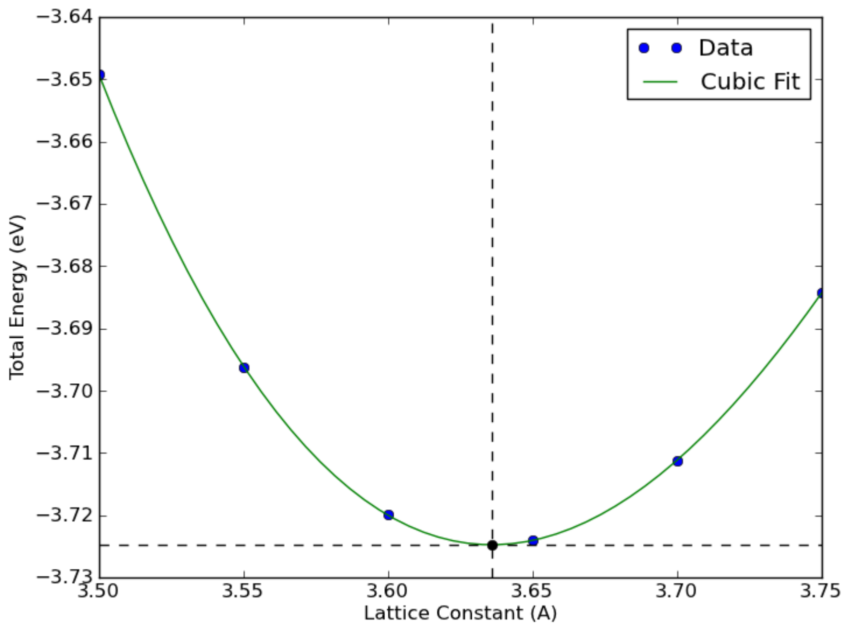
Placed in the repository: dft-revised.pdf

3 Problem 4

```python
import numpy as np
import matplotlib.pyplot as plt

data_y = [-3.649238, -3.696204, -3.719946, -3.723951, -3.711284, -3.68426]
data_x = [3.5, 3.55, 3.6, 3.65, 3.7, 3.75]

pfit = np.polyfit(data_x, data_y, 3)
pder = np.polyder(pfit)
pder_roots = np.roots(pder)
en_roots = np.polyval(pfit, pder_roots)
pdouble_der = np.polyder(pder)

en_ext = np.polyval(pdouble_der, pder_roots)

for i in range(2):
    if(en_ext[i]>0):
        lat_const_min = pder_roots[i]
        energy_min = en_roots[i]

print 'Equilibrium Lattice Constant: {0} Angstrom'.format(lat_const_min)
print 'Minimum Energy: {0} eV'.format(energy_min)

pfit_x = np.linspace(data_x[0], data_x[-1])
pfit_plot = np.polyval(pfit,pfit_x)

plt.plot(data_x, data_y, marker='o', linestyle='none')
plt.plot(pfit_x, pfit_plot)
plt.axvline(x = lat_const_min, linestyle='--', color='k')
plt.axhline(y = energy_min, linestyle='--', color='k')
plt.plot(lat_const_min, energy_min, 'ko')
plt.xlabel('Lattice Constant (A)')
plt.ylabel('Total Energy (eV)')
plt.legend(['Data', 'Cubic Fit'], loc='best')
plt.savefig('hw1_q4.png')
plt.show()
```

```
Equilibrium Lattice Constant: 3.63579751533 Angstrom
Minimum Energy:  -3.72475331358 eV
```

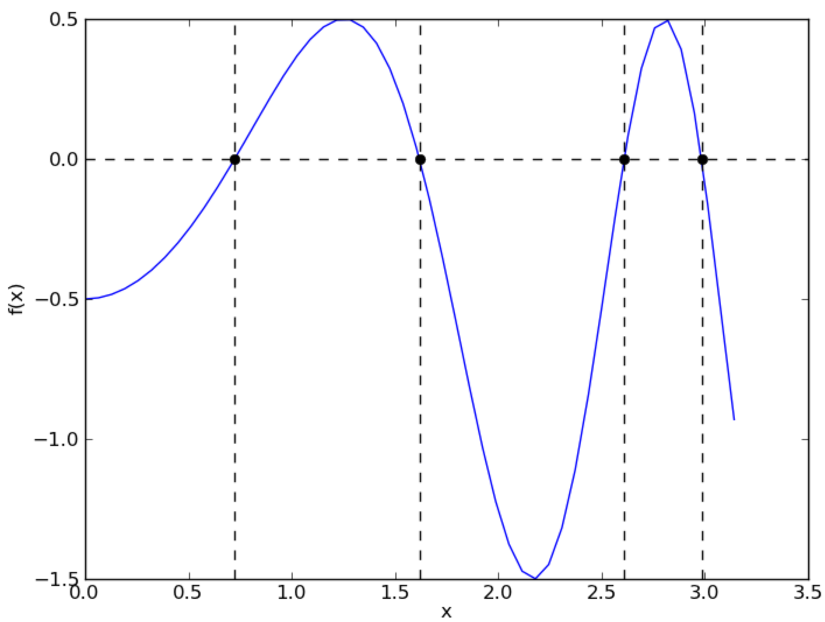


4 Problem 5

```
import numpy as np
from scipy.optimize import fsolve
import matplotlib.pyplot as plt

def f(x):
    y = np.sin(x**2) - 0.5
    return y

x0 = [0.75, 1.5, 2.3, 3]
x_soln = fsolve(f, x0)

print 'Roots for the range [0,pi]: {0}'.format(x_soln)

x1 = np.linspace(0,np.pi)
y1 = f(x1)

plt.plot(x1, y1)
plt.axvline(x = x_soln[0], linestyle='--', color='k')
plt.axvline(x = x_soln[1], linestyle='--', color='k')
plt.axvline(x = x_soln[2], linestyle='--', color='k')
plt.axvline(x = x_soln[3], linestyle='--', color='k')
plt.axhline(y = 0, linestyle='--', color='k')
plt.plot(x_soln, f(x_soln), 'ko')
```

```
plt.xlabel('x')
plt.ylabel('f(x)')
plt.savefig('hw1_q5.png')
plt.show()
```

```
Roots for the range [0,pi]:  [ 0.72360125  1.61802159  2.60898143  2.9834844 ]
```



5 Problem 6

```
import numpy as np
import numpy.linalg as la

A = np.array([[1, -3, 9, -27], [1, -1, 1, -1], [1, 1, 1, 1], [1, 2, 4, 8]])
b = np.array([-2, 2, 5, 1])

print 'Solution from linear algebra and python:\n {0}'.format(la.solve(A, b))
print 'Solution from linear algebra:\n {0}'.format(np.dot(la.inv(A), b))
print 'They match eachother'
```

```
Solution from linear algebra and python:
 [ 4.65        1.84166667  -1.15        -0.34166667]
```

```
Solution from linear algebra:
 [ 4.65        1.84166667  -1.15        -0.34166667]
They match eachother
```