

schroedingerCubic

March 2, 2021

1 Problem 1 Part a

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[1]: import numpy as np
import matplotlib.pyplot as plt
import scipy.integrate
import scipy.optimize
from scipy.optimize import root as rootFinder
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[2]: class Schroedinger :

    def __init__(self) :
        self.hbar = 1.0          # Planck's constant / 2pi
        self.m = 1.0             # particle mass
        self.omega = 1.0         # oscillator frequency
        self.E = 0.0             # current energy in search
        self.N = 500             # number of lattice points = N+1
        self.x_left = -7.0       # left boundary
        self.x_right = 7.0       # right boundary
        self.h = (self.x_right - self.x_left) / self.N # grid spacing
        self.xvals = np.linspace(self.x_left, self.x_right, self.N+1) # x value

    ↪ for phi
        self.phi_left = np.zeros(self.N+1) # wave function integrating from
    ↪ left
        self.phi_right = np.zeros(self.N+1) # wave function integrating from
    ↪ right
        self.phi = np.zeros(self.N+1)      # whole wave function
        self.i_match = 0                   # Index of turning point
        self.x_match = 0.                  # Turning point x value
        self.sign = 1                      # current sign used to make F(E)

    ↪ continuous
        self.nodes = 0                    # current number of nodes in
    ↪ wavefunction

    def V(self, x):                     # harmonic oscillator potential
        return 0.5 * self.m * self.omega**2 * (x**2 + (1/20)*x**3)
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def q(self, x):
    # Sturm-Liouville q function
    return 2 * self.m / self.hbar**2 * (self.E - self.V(x))

def F(self, energy):
    # eigenvalue at F(E) = 0

    # set energy needed by the q(x) function
    self.E = energy

    # find the right turning point
    self.i_match = self.N

    x = self.x_right
    # start at right boundary
    while self.V(x) > self.E:
        # in forbidden region
        self.i_match -= 1
        x -= self.h
        if self.i_match < 0:
            raise Exception("can't find right turning point")
    self.x_match = self.xvals[ self.i_match ]

    # integrate self.phi_left using Numerov algorithm
    self.phi_left[0] = 0.0
    self.phi_left[1] = 1.0e-10
    c = self.h**2 / 12.0
    # constant in Numerov formula
    for i in range(1, self.i_match+1):
        x = self.x_left + i * self.h
        self.phi_left[i+1] = 2 * (1 - 5 * c * self.q(x)) * self.phi_left[i]
        self.phi_left[i+1] -= (1 + c * self.q(x - self.h)) * self.
→phi_left[i-1]
        self.phi_left[i+1] /= 1 + c * self.q(x + self.h)

    # integrate self.phi_right
    self.phi[self.N] = self.phi_right[self.N] = 0.0
    self.phi[self.N-1] = self.phi_right[self.N-1] = 1.0e-10
    for i in range(self.N - 1, self.i_match - 1, -1):
        x = self.x_right - i * self.h
        self.phi_right[i-1] = 2 * (1 - 5 * c * self.q(x)) * self.
→phi_right[i]
        self.phi_right[i-1] -= (1 + c * self.q(x + self.h)) * self.
→phi_right[i+1]
        self.phi_right[i-1] /= 1 + c * self.q(x - self.h)
        self.phi[i-1] = self.phi_right[i-1]

    # rescale self.phi_left
    scale = self.phi_right[self.i_match] / self.phi_left[self.i_match]

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for i in range(self.i_match + 2):
    self.phi_left[i] *= scale
    self.phi[i] = self.phi_left[i]

# make F(E) continuous
# count number of nodes in self.phi_left
n = 0
for i in range(1, self.i_match+1):
    if self.phi_left[i-1] * self.phi_left[i] < 0.0:
        n += 1

# flip its sign when a new node develops

if n != self.nodes:
    self.nodes = n
    self.sign = -self.sign

return ( self.sign *
        ( self.phi_right[self.i_match-1] - self.phi_right[self.i_match+1] -
          self.phi_left [self.i_match-1] + self.phi_left[self.i_match+1] ) /
        (2 * self.h * self.phi_right[self.i_match]) )

def normalize(self):
    norm = 0.0
    norm = np.sqrt( np.sum( self.phi**2 ) / self.N )
    self.phi = self.phi / norm

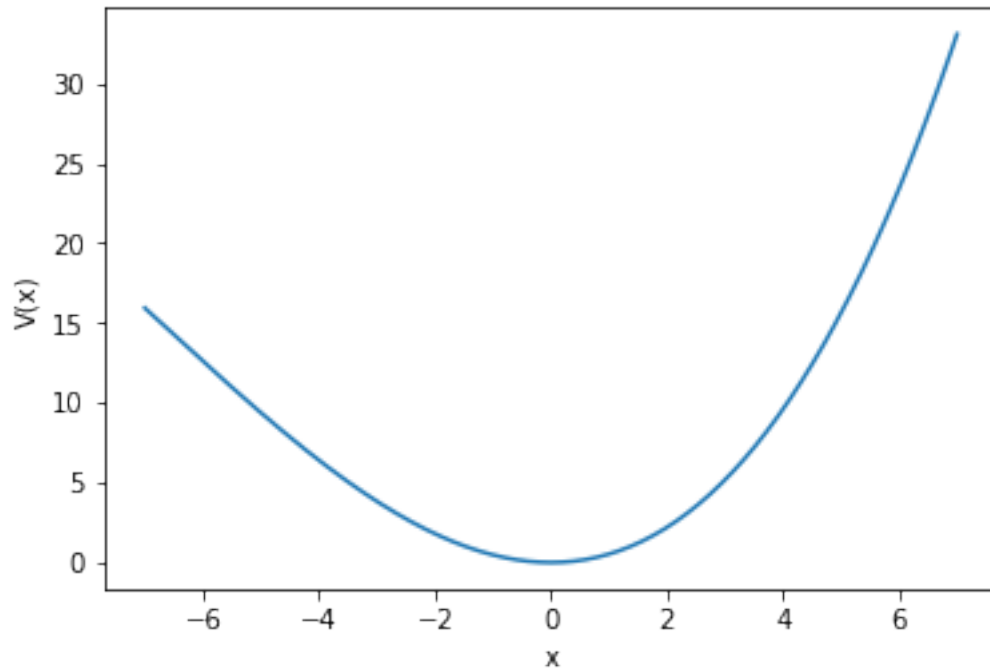
```

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[3]: schroedinger = Schroedinger()

x = schroedinger.x_left + schroedinger.h * np.linspace(0, schroedinger.N, ↵
↪schroedinger.N+1)
vx = schroedinger.V(x)
plt.plot(x,vx)
plt.xlabel("x")
plt.ylabel("V(x)")
plt.show()

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[4]: # find the energy levels
E_max = 5.0
schroedinger.E = 0.1      # guess an E below the ground state
level = 0                 # level number
E_old = 0.0               # previous energy eigenvalue

while True:               # loop over levels

    # estimate next E and dE
    dE = 0.5 * (schroedinger.E - E_old)
    E_old = schroedinger.E
    schroedinger.E += dE

    res = rootFinder( schroedinger.F,
                       x0=schroedinger.E)
    #                               x1=schroedinger.E+dE )
    schroedinger.E = res.x

    level += 1

    res = rootFinder( schroedinger.q,
                       x0=schroedinger.x_left)
    #                               x1=schroedinger.x_match )
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x = res.x
#swrite = '-: {0:4.2f} {1:4.2f}'.format( x, schroedinger.E )
#print (swrite)

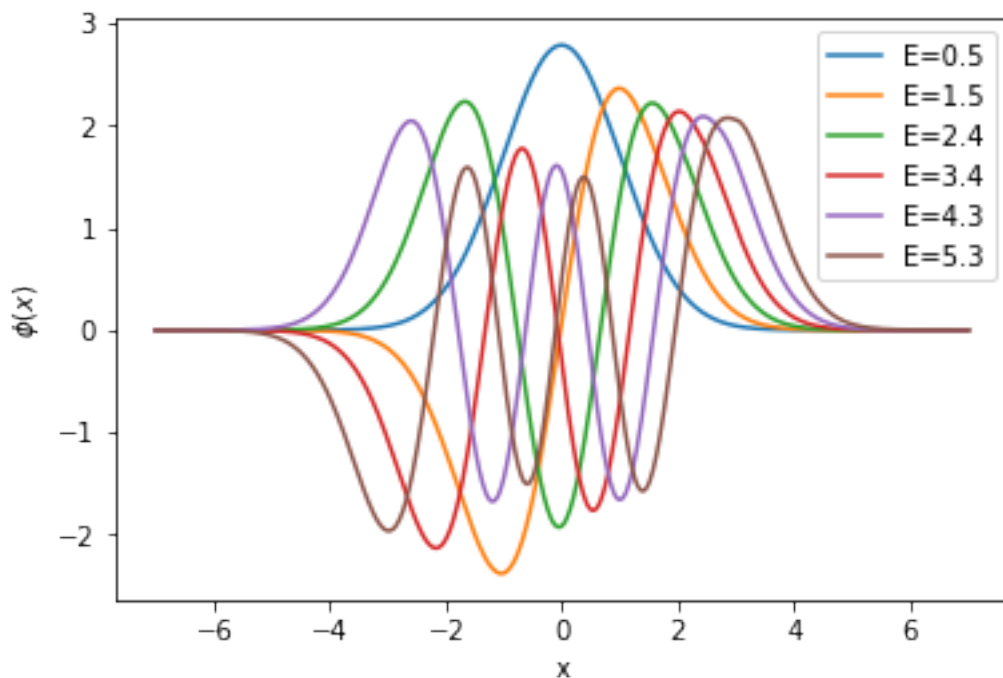
res = rootFinder( schroedinger.q,
                  x0=schroedinger.x_match)
#                  x1=schroedinger.x_right )
x = res.x
#swrite = '+: {0:4.2f} {1:4.2f}'.format( x, schroedinger.E )
#print (swrite)

schroedinger.normalize()
xvals = schroedinger.x_left + schroedinger.h * np.arange(schroedinger.N+1)

plt.plot(xvals, schroedinger.phi, label="E=%2.1f" % (schroedinger.E) )

if schroedinger.E >= E_max:      # we are done
    break
plt.legend()
plt.xlabel("x")
plt.ylabel(r"$\phi(x)$")
plt.show()

```



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[5]: %matplotlib notebook
      # print the search function
      schroedinger.E = 0.1
      dE = 0.01
      E_data = []
      F_data = []
      while schroedinger.E < E_max:
          E_data.append( schroedinger.E )
          F_data.append( schroedinger.F(schroedinger.E) )
          schroedinger.E += dE

      plt.plot(E_data,F_data)
      plt.ylim(-10,10)
      plt.xlabel("E")
      plt.ylabel("F(E)")
      plt.axhline(linewidth=1, color='k')
      plt.show()
```

<IPython.core.display.Javascript object>

<IPython.core.display.HTML object>

[]: