

Q3_ass7

November 22, 2021

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[4]: %run lib.ipynb
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[5]: def shooting_method(d2ydx2, dydx, x0, y0, xf, yf, z_guess1, z_guess2, h,
    →tol=1e-6):
    →Lower boundary value of x, y0 = y(x0)
    →Upper boundary value of x, yf = y(xf)
    →dy/dx
    x, y, z = runge_kutta(d2ydx2, dydx, x0, y0, z_guess1, xf, h)
    yn = y[-1]

    if abs(yn - yf) > tol:
        if yn < yf:
            z_l = z_guess1
            yl = yn

            x, y, z = runge_kutta(d2ydx2, dydx, x0, y0, z_guess2, xf, h)
            yn = y[-1]

            if yn > yf:
                z_h = z_guess2
                yh = yn

                # calculate zeta using Lagrange interpolation
                zeta = lagrange_interpolation(z_h, z_l, yh, yl, yf)

                # using this zeta to solve using RK4
                x, y, z = runge_kutta(d2ydx2, dydx, x0, y0, zeta, xf, h)
                return x, y, z

        else:
            print("Bracketing failed. Change your set of guesses.")

    elif yn > yf:
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        z_h = z_guess1
        y_h = y_n

        x, y, z = runge_kutta(d2ydx2, dydx, x0, y0, z_guess2, xf, h)
        y_n = y[-1]

        if y_n < y_f:
            z_l = z_guess2
            y_l = y_n

            # calculate zeta using Lagrange interpolation
            zeta = lagrange_interpolation(z_h, z_l, y_h, y_l, y_f)

            x, y, z = runge_kutta(d2ydx2, dydx, x0, y0, zeta, xf, h)
            return x, y, z

        else:
            print("Bracketing failed. Change your set of guesses.")

    else:
        return x, y, z          # bang-on solution with z_guess1

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[6]: #Q3
      # solv Schrodinger Equation

      def ad2ydt2(t, y, z):    #ground state
          return -(math.pi**2)*y/4

      def bd2ydt2(t, y, z): #excited state
          return -(math.pi**2)*y

      def dydt(t, y, z):
          return z

      # Define boundary values
      t_i = 0
      t_f = 2
      y_i = 0
      y_f = 0

      t, y, z = shooting_method(ad2ydt2, dydt, t_i, y_i, t_f, y_f, -2, 10, h=0.1)

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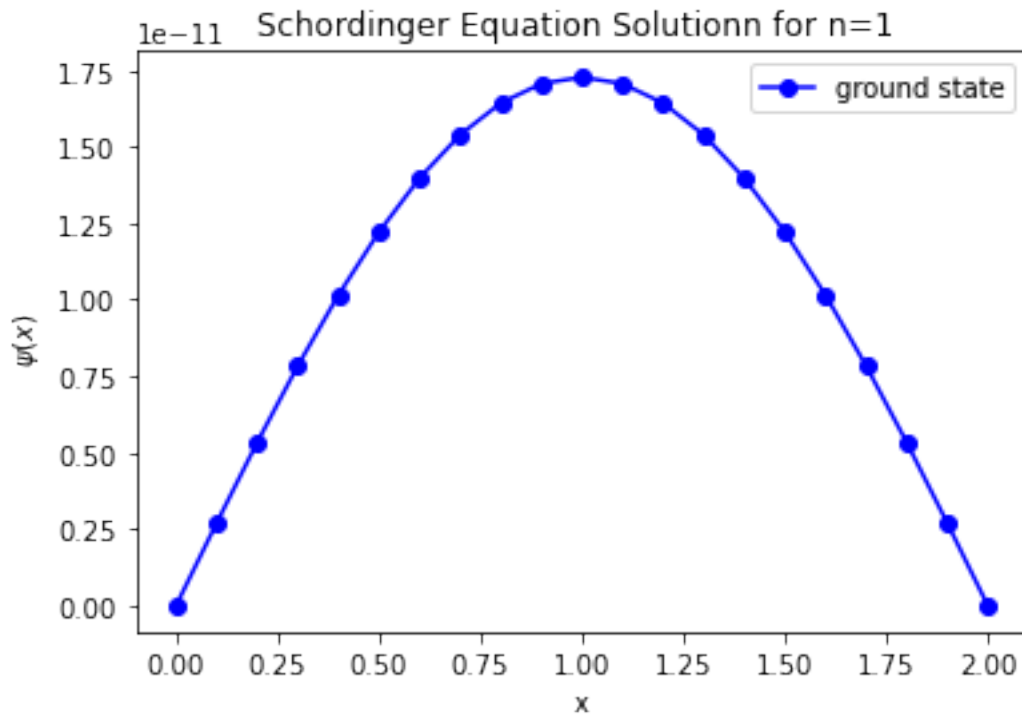
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plt.plot(t,y,'b-o',label='ground state')
plt.xlabel('x')
plt.ylabel('  $\psi(x)$  ')
plt.title('Schordinger Equation Solutionn for n=1 ')
plt.legend()
plt.show()

t, y, z = shooting_method(bd2ydt2, dydt, t_i, y_i, t_f, y_f, -2, 10, h=0.1)

plt.plot(t,y,'r-o',label='excited state' )
plt.xlabel('x')
plt.ylabel('  $\psi(x)$  ')
plt.title('Schordinger Equation Solution for n=2 ')
plt.legend()

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[6]: <matplotlib.legend.Legend at 0x7ff4e2e3ed30>

