Homework 10

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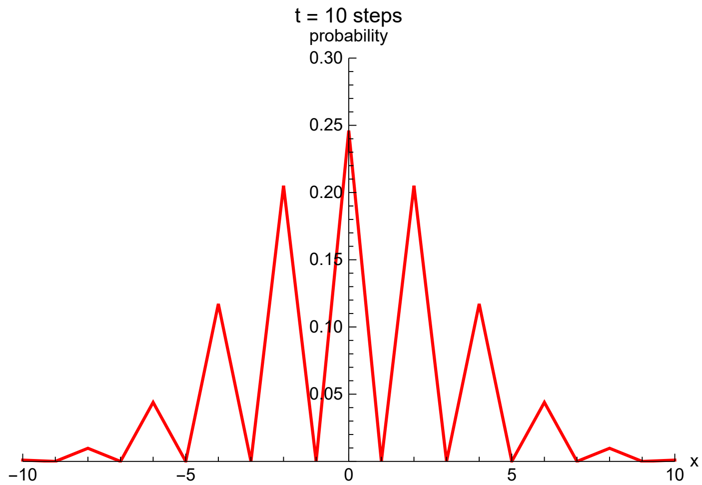
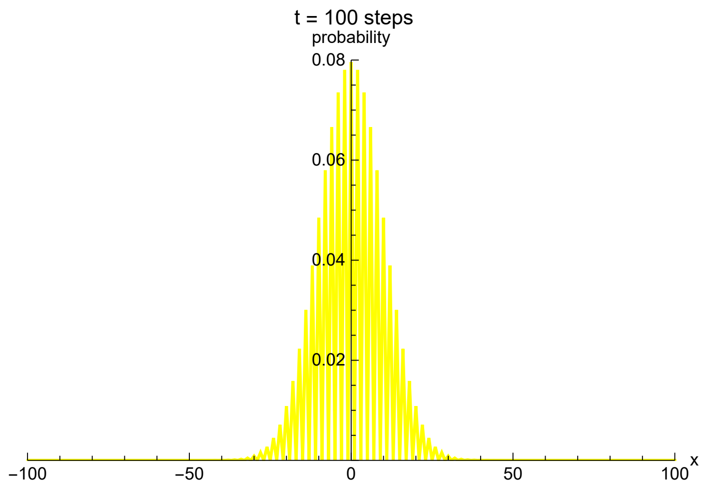
Problem 1: Fig 7.12

In[ ]:=
```
ClearAll["Global`*"];
t = 11;
P = Table[0, {i, -10, 10, 1}, {j, 1, t, 1}];
(*starting from the origin*)
P[[11, 1]] = 1;
Do[Do[P[[i, n]] = 0.5 * (P[[i - 1, n - 1]] + P[[i + 1, n - 1]]);
   P[[1, n]] = 0.5 * P[[2, n - 1]];
   P[[21, n]] = 0.5 * P[[20, n - 1]], {i, 2, 20}], {n, 2, t}];
pp = Table[0, {i, 21}];
Do[
  pp[[i]] = {i - 11, P[[i, t]]}, {i, 1, 21, 1}];
p1 = ListPlot[pp, PlotRange → {{-10, 10}, {0, 0.3}}, PlotLabel → "t = 10 steps",
  AxesLabel → {"x", "probability"}, Joined → {True}, PlotStyle → Red]
(*The 100 steps case*)
t1 = 101;
P1 = Table[0, {i, -100, 100, 1}, {j, 1, t1, 1}];
P1[[101, 1]] = 1;
Do[
  Do[
   P1[[i, n]] = 0.5 * (P1[[i - 1, n - 1]] + P1[[i + 1, n - 1]]);
   P1[[1, n]] = 0.5 * P1[[2, n - 1]];
   P1[[201, n]] = 0.5 * P1[[200, n - 1]], {i, 2, 200}], {n, 2, t1}];
pp1 = Table[0, {i, 201}];
Do[
  pp1[[i]] = {i - 101, P1[[i, t1]]}, {i, 1, 201, 1}];
p11 = ListPlot[pp1, PlotLabel → " t = 100 steps", AxesLabel → {"x", "probability"},
  PlotRange → {{-100, 100}, {0, 0.08}}, Joined → {True}, PlotStyle → Yellow]
```

Out[•]=



Out[•]=



Problem 2: 10.1

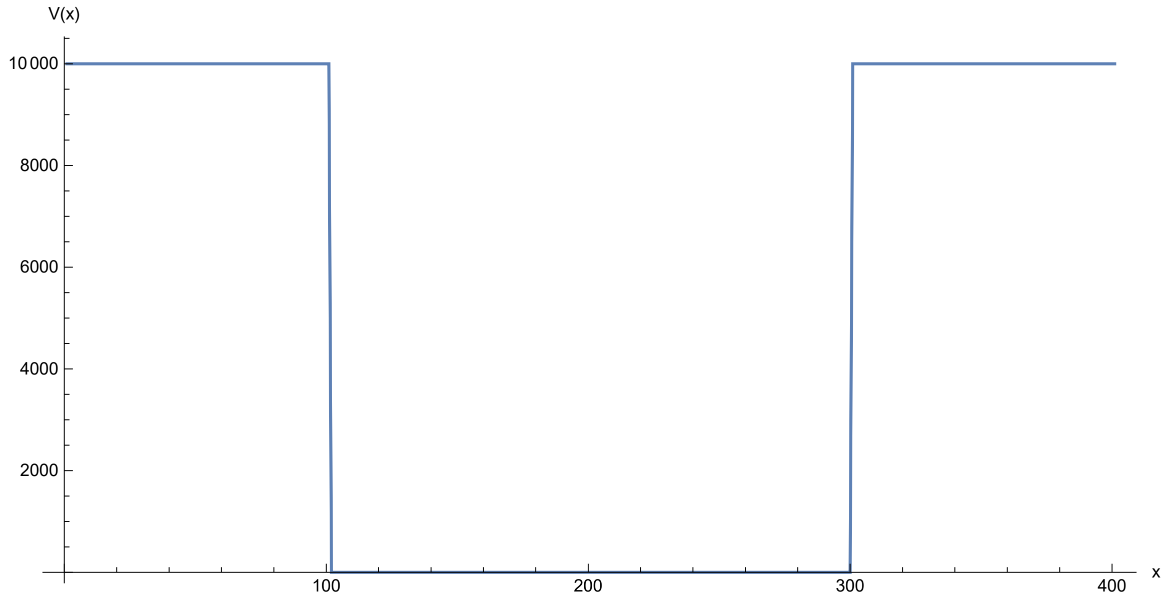
```
(*The odd solution*)
ClearAll["Global`*"]
xMax = 2.0; dx = 0.01;
x = Range[-xMax, xMax, dx]; lx = Length[x];
v = Table[0.0, {i, lx}];
potEng = 10000.0;

Do[
  If[x[[i]] <= -1.0, v[[i]] = potEng];
  If[x[[i]] >= 1.0, v[[i]] = potEng];
  If[x[[i]] == 0.0, i0 = i]; (* i0 = central position of the well *)
  , {i, lx}];
nEng = 5; (* number of energy levels *)
color = {Red, Yellow, Orange, Green, Magenta};
labels = {"En0", "En1", "En2", "En3", "En4"};
engOddList = Table[0.0, {i, nEng}];
plot = Table[0.0, {i, nEng}];
```

```
eng = 1.0; (* first guess for E *)
psiMax = 2.0; (* top bound for psi *)

Do[
  dE = .4; (* first guess for dE *)

  (* Obtaining the sign of the initial psi RIGHT*)
  psi = Table[0.0, {i, lx}];
  psi[[i0]] = 0.0; psi[[i0 - 1]] = -dx * j;  (* δx slope at x = 0 and 0.0 ψ at x=0*)
  i = i0 + 1;
  While[Abs[psi[[i - 1]]] < psiMax && i < lx,
   psi[[i]] =
    2.0 psi[[i - 1]] - psi[[i - 2]] - 2.0 (eng - v[[i - 1]]) psi[[i - 1]] dx^2;  i++];
  psiLastR = psi[[i - 1]] ; (* Last value of psi before quitting *)

  (* Main loop for energy levels *)
  While[Abs[dE] > 0.000000000001,
   psi = Table[0.0, {i, lx}];
   psi[[i0]] = 0.0; psi[[i0 - 1]] = -dx * j;
   psi[[i0 + 1]] = dx * j;  (* δx slope at x = 0 and 0.0 ψ at x=0*)

   (*multiply dx by J as a systematic way
     for increasing the slope of ψ around x=0 with higher E values,
   to accomodate higher slopes for increasing E values and avoid the probability
    amplitudes falling off with larger E's as the frequncies increase*)

   i = i0 + 2;
   While[Abs[psi[[i - 1]]] < psiMax && i < lx,
    psi[[i]] =
     2.0 psi[[i - 1]] - psi[[i - 2]] - 2.0 (eng - v[[i - 1]]) psi[[i - 1]] dx^2;  i++];
   psiNewR = psi[[i - 1]] ;
   If[Sign[psiNewR] == Sign[psiLastR], eng = eng + dE];
   If[Sign[psiNewR] != Sign[psiLastR], dE = -dE / 2.0; eng = eng + dE];
   psiLastR = psiNewR];
  (*-----------------------------------------------------------------------*)

  dEl = 0.4;
  While[Abs[dEl] > 0.000000000001,
   k = i0 - 2;
   While[Abs[psi[[k + 1]]] < psiMax && k > 0,
    psi[[k]] =
     2.0 psi[[k + 1]] - psi[[k + 2]] - 2.0 (eng - v[[k + 1]]) psi[[k + 1]] dx^2;  k--];
   psiNewL = psi[[k + 1]] ;
   If[Sign[psiNewL] == Sign[psiLastL], eng = eng - dEl];
   (*used negative here to reverse direction*)
   If[Sign[psiNewL] != Sign[psiLastL], dEl = -dEl / 2.0; eng = eng + dEl];
   psiLastL = psiNewL];

  (*-----------------------------------------------------------------------*)
```

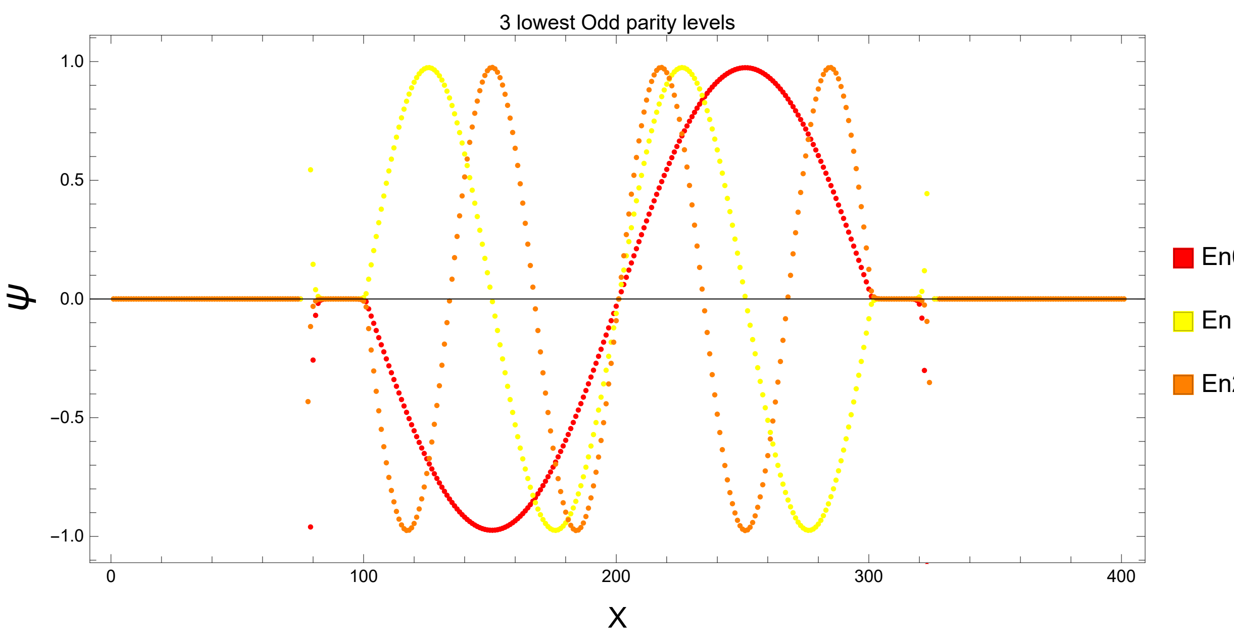
```
  engOddList[[j]] = eng;
  eng = eng + 0.5;

  (*divide ψ by 0.328, which is the amplitude we found before normalization*)

  plot[[j]] =
   ListPlot[psi / 0.328, PlotRange → All, PlotStyle → {color[[j]], PointSize → 0.005},
    PlotLegends → SwatchLegend[{color[[j]]}, {labels[[j]]}]]
  , {j, nEng}];


leg = SwatchLegend[{Red, Yellow, Orange}, {"E0", "E1", "E2"}];
engOddList (* Calculations using shooting method *);
engExact = Table[((2.0 n) Pi / 2.0)^2 / 2.0, {n, 5}] ;

(* Exact .. corrected, since the odd functions have
 different integers or half integers of pi in their equation*)
ListPlot[v, Joined → True, AxesLabel → {"x", "V(x)"}, AspectRatio → 0.5, ImageSize → 600]
Show[plot[[1]], plot[[2]], plot[[3]], PlotRange → {-1, 1},
 AspectRatio → 0.5, ImageSize → 600, Frame → True,
 FrameLabel → {Style["X", FontSize → 15], Style["ψ", FontSize → 20]},
 PlotLabel → "3 lowest Odd parity levels"]

Print["Exact Energies for the first 5 odd levels are:\n " <> ToString [engExact] <>
  "\nestimated values from computations using the shooting method were:\n" <>
  ToString[engOddList]]
(*------------------------------------------------------------------------*)
(*------------------------------------------------------------------------*)
(*The even solution*)
ClearAll["Global`*"]
xMax = 2.0; dx = 0.01;
x = Range[-xMax, xMax, dx]; lx = Length[x];
v = Table[0.0, {i, lx}];
potEng = 10000.0;
Do[
  If[x[[i]] <= -1.0, v[[i]] = potEng];
  If[x[[i]] >= 1.0, v[[i]] = potEng];
  If[x[[i]] == 0.0, i0 = i]; (* i0 = central position of the well *)
  , {i, lx}];
nEng = 5; (* number of energy levels *)
engEvenList = Table[0.0, {i, nEng}];
plot = Table[0.0, {i, nEng}];

eng = 1.0; (* first guess for E *)
psiMax = 2.0; (* top bound for psi *)

Do[
  dE = .4; (* first guess for dE *)
```

```
  (* Obtaining the sign of the initial psi *)
  psi = Table[0.0, {i, lx}];
  psi[[i0]] = 1.0; psi[[i0 - 1]] = 1.0;  (* zero slop at x = 0 *)
  i = i0 + 1;
  While[Abs[psi[[i - 1]]] < psiMax && i < lx,
   psi[[i]] =
    2.0 psi[[i - 1]] - psi[[i - 2]] - 2.0 (eng - v[[i - 1]]) psi[[i - 1]] dx^2;  i++];
  psiLast = psi[[i - 1]] ; (* Last value of psi before quitting *)

  (* Main loop for energy levels *)
  While[Abs[dE] > 0.000000000001,
   psi = Table[0.0, {i, lx}];
   psi[[i0]] = 1.0; psi[[i0 - 1]] = 1.0;  (* zero slop at x = 0 *)
   i = i0 + 1;
   While[Abs[psi[[i - 1]]] < psiMax && i < lx,
    psi[[i]] =
     2.0 psi[[i - 1]] - psi[[i - 2]] - 2.0 (eng - v[[i - 1]]) psi[[i - 1]] dx^2;  i++];
   psiNew = psi[[i - 1]] ;
   If[Sign[psiNew] == Sign[psiLast], eng = eng + dE];
   If[Sign[psiNew] != Sign[psiLast], dE = -dE / 2.0; eng = eng + dE];
   psiLast = psiNew];
  engEvenList[[j]] = eng;
  eng = eng + 0.5;
  plot[[j]] = ListPlot[psi, PlotRange → All]
  , {j, nEng}];

(* Results *)
engExact = Table[((2.0 n - 1) Pi / 2.0)^2 / 2.0, {n, 5}] (* Exact *)
Print["Exact Energies for the first 5 even levels are:\n " <> ToString [engExact] <>
  "\nestimated values from computations using the shooting method were:\n" <>
  ToString[engEvenList]]
engEvenList (* Calculations using shooting method *)

ListPlot[v, Joined → True, AxesLabel → {"x", "V(x)"}];
Show[plot[[1]], plot[[2]], PlotRange → {-1, 1}]
```

Out[ ]=



Out[ ]=



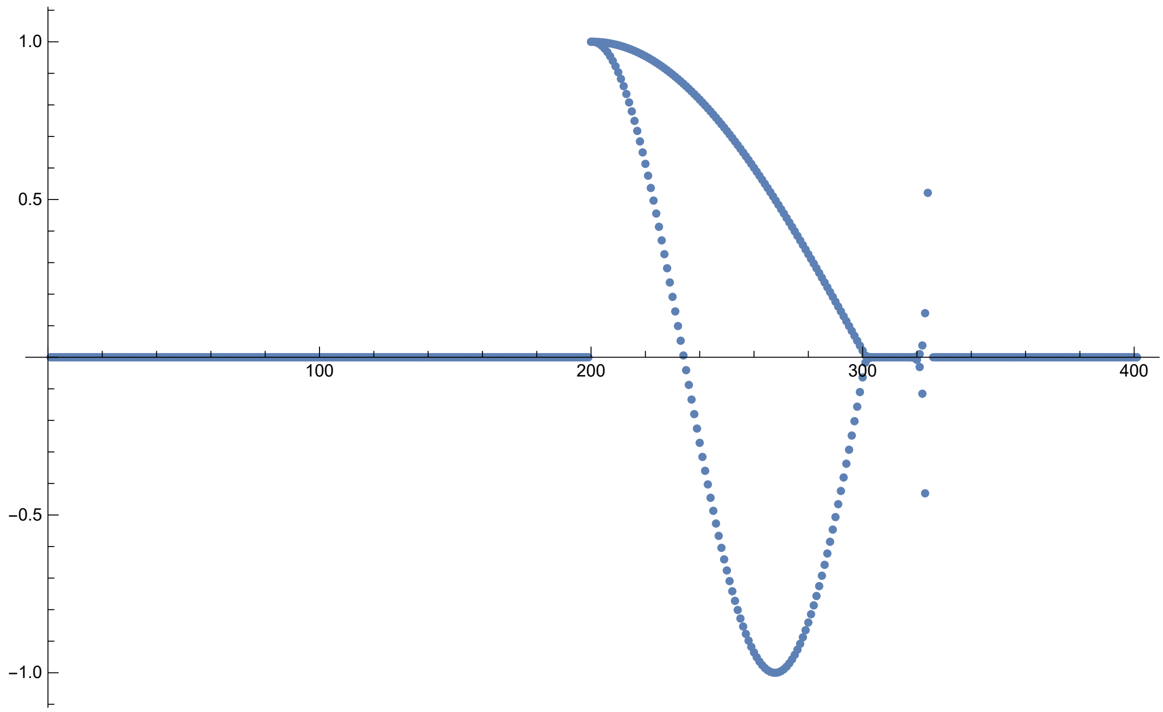

```
Exact Energies for the first 5 odd levels are:
 {4.9348, 19.7392, 44.4132, 78.9568, 123.37}
estimated values from computations using the shooting method were:
{4.89847, 19.5891, 44.0575, 78.2796, 122.222}
```

Out[ ]= {1.2337, 11.1033, 30.8425, 60.4513, 99.9297}

```
Exact Energies for the first 5 even levels are:
 {1.2337, 11.1033, 30.8425, 60.4513, 99.9297}
estimated values from computations using the shooting method were:
{1.21258, 10.9115, 30.2999, 59.3589, 98.0605}
```

Out[ ]= {1.21258, 10.9115, 30.2999, 59.3589, 98.0605}

Out[ ]=



Problem 3: 10.2

```
(*I solved the problem using the shotting because I couldn't
 solve using the matching at first. But then I solved using both. *)
(*Firstly using hte matching method energy*)
(*First energy*)
ClearAll["Global`*"];
dx = 0.01; xMin = -4; xMax = 4;
x = Range[xMin, xMax, dx]; lx = Length[x];
eng = 0.45; (* first guess for E *)

dE = .02; (* first guess for dE *)

vLJ[x_, m_, w_] := 1/2 * m * w^2 * x^2;
v = Table[1/2 i^2, {i, -xMax, xMax, dx}]; (* harmonic potential *)
iMin = Position[v, Min[v]][[1, 1]]; (* Minimum potential position *)

iOverLap = 20; (* determines number of overlapping steps *)
(* Initialization of ψL and ψR;
ψL runs from the beginging of x to iOverLap
 steps beyond the minimum position of the potential;
ψR runs iOverLap steps before the minimum till the end;
 ψL and ψR overlaps on 2 × iOverLap points on the x axis;
```

```
 *)
psiL = Table[0.0, {i, iMin + iOverLap}];
lL = Length[psiL];
psiR = Table[0.0, {i, iMin - iOverLap, lx}];
lR = Length[psiR];

(* Start with a small slope by giving the following values to the first elements in each
 psi. We keep the second elements zeros. So we start from the third elements *)
psiL[[1]] = -0.0001 dx; psiR[[1]] = psiL[[1]];

(* Obtaining the slopes of the initial psi *)

Do[psiL[[i]] = 2.0 psiL[[i - 1]] - psiL[[i - 2]] - 2.0 (eng - v[[i - 1]]) psiL[[i - 1]] dx^2
  , {i, 3, lL}];
Do[psiR[[i]] = 2.0 psiR[[i - 1]] - psiR[[i - 2]] - 2.0 (eng - v[[1 - i]]) psiR[[i - 1]] dx^2
  , {i, 3, lR}]; (* v is reversed: not i - 1, but -(i - 1) *)
psiR = Reverse[psiR]; (* reverse the elements of ψR to the right order *)
psiR = psiR / Sqrt[psiR.psiR * dx]; (*the normalization*)
(* Scaling: ψL = ψR at the minimum position of v *)
psiL = psiL psiR[[iOverLap]] / psiL[[iMin]];

(* Slopes calculations: Slope ≡ difference, since dx is the same *)
sL = psiL[[iMin + 1]] - psiL[[iMin - 1]];
sR = psiR[[iOverLap + 1]] - psiR[[iOverLap - 1]];
ds = sL - sR;
signo = Sign[ds];
While[Abs[dE] > 0.000000000001,
  Do[psiL[[i]] = 2.0 psiL[[i - 1]] - psiL[[i - 2]] - 2.0 (eng - v[[i - 1]]) psiL[[i - 1]] dx^2
   , {i, 3, lL}];
  Do[
   psiR[[i]] = 2.0 psiR[[i - 1]] - psiR[[i - 2]] - 2.0 (eng - v[[1 - i]]) psiR[[i - 1]] dx^2
   , {i, 3, lR}]; (* v is reversed: not i - 1, but -(i - 1) *)
  psiR = Reverse[psiR]; (* reverse the elements of ψR to the right order *)
  psiR = psiR / Sqrt[psiR.psiR * dx]; (*the normalization*)
  psiL = psiL psiR[[iOverLap]] / psiL[[iMin]];
  sL = psiL[[iMin + 1]] - psiL[[iMin - 1]];
  sR = psiR[[iOverLap + 1]] - psiR[[iOverLap - 1]];
  xpsiL = Table[{x[[i]], psiL[[i]]}, {i, lL}];
  xpsiR = Table[{x[[i + lx - lR]], psiR[[i]]}, {i, lR}];
  ds = sL - sR;
  signn = Sign[ds];



  If[Sign[signn] == Sign[signo], eng = eng + dE];
  If[Sign[signn] != Sign[signo], dE = -dE / 2.0; eng = eng + dE];
  signo = signn];
```

```
eng
```

```
p1 = ListPlot[xpsiL, PlotStyle → Black, Joined → True];
p2 = ListPlot[xpsiR, PlotStyle → Red, Joined → True];
Show[p1, p2, PlotRange → All, AxesLabel → {"x", "ψ"}]
ListPlot[v, PlotRange → {{-10, 20}}, AxesLabel → {"x", "V(x)"}]
```

```
(*Second energy*)
ClearAll["Global`*"];
dx = 0.01; xMin = -5; xMax = 5;
x = Range[xMin, xMax, dx]; lx = Length[x];
eng = 1.4; (* first guess for E *)

dE = .001; (* first guess for dE *)

vLJ[x_, m_, w_] := 1/2 * m * w^2 * x^2;
v = Table[1/2 i^2, {i, -xMax, xMax, dx}]; (* harmonic potential *)
iMin = Position[v, Min[v]][[1, 1]]; (* Minimum potential position *)

iOverLap = 20; (* determines number of overlapping steps *)
(* Initialization of ψL and ψR;
ψL runs from the beginging of x to iOverLap
 steps beyond the minimum position of the potential;
ψR runs iOverLap steps before the minimum till the end;
 ψL and ψR overlaps on 2 × iOverLap points on the x axis;
 *)
psiL = Table[0.0, {i, iMin + iOverLap}];
lL = Length[psiL];
psiR = Table[0.0, {i, iMin - iOverLap, lx}];
lR = Length[psiR];

(* Start with a small slope by giving the following values to the first elements in each
 psi. We keep the second elements zeros. So we start from the third elements *)
psiL[[1]] = -0.0001 dx; psiR[[1]] = psiL[[1]];

(* Obtaining the slopes of the initial psi *)

Do[psiL[[i]] = 2.0 psiL[[i - 1]] - psiL[[i - 2]] - 2.0 (eng - v[[i - 1]]) psiL[[i - 1]] dx^2
  , {i, 3, lL}];
Do[psiR[[i]] = 2.0 psiR[[i - 1]] - psiR[[i - 2]] - 2.0 (eng - v[[1 - i]]) psiR[[i - 1]] dx^2
  , {i, 3, lR}]; (* v is reversed: not i - 1, but -(i - 1) *)
psiR = Reverse[psiR]; (* reverse the elements of ψR to the right order *)
```

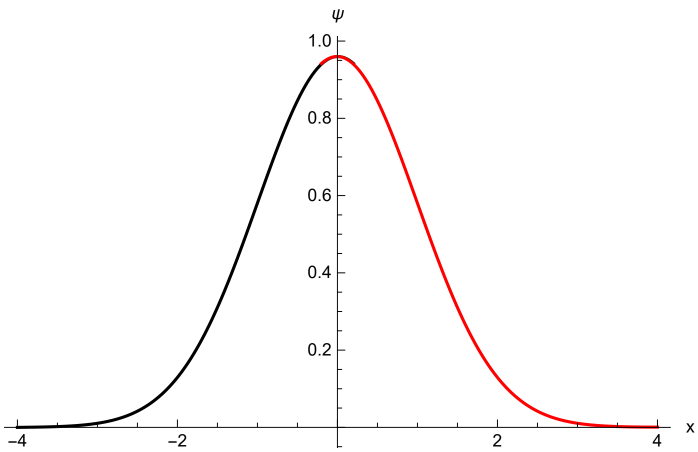
```
psiR = psiR / Sqrt[psiR.psiR * dx]; (*the normalization*)
(* Scaling: ψL = ψR at the minimum position of v *)
psiL = psiL psiR[[iOverLap]] / psiL[[iMin]];

(* Slopes calculations: Slope ≡ difference, since dx is the same *)
sL = psiL[[iMin + 1]] - psiL[[iMin - 1]];
sR = psiR[[iOverLap + 1]] - psiR[[iOverLap - 1]];
ds = sL - sR;
signo = Sign[ds];
While[Abs[dE] > 0.000000000001,
  Do[psiL[[i]] = 2.0 psiL[[i - 1]] - psiL[[i - 2]] - 2.0 (eng - v[[i - 1]]) psiL[[i - 1]] dx^2
   , {i, 3, lL}];
  Do[
   psiR[[i]] = 2.0 psiR[[i - 1]] - psiR[[i - 2]] - 2.0 (eng - v[[1 - i]]) psiR[[i - 1]] dx^2
   , {i, 3, lR}]; (* v is reversed: not i - 1, but -(i - 1) *)
  psiR = Reverse[psiR]; (* reverse the elements of ψR to the right order *)
  psiR = psiR / Sqrt[psiR.psiR * dx]; (*the normalization*)
  psiL = psiL psiR[[iOverLap]] / psiL[[iMin]];
  sL = psiL[[iMin + 1]] - psiL[[iMin - 1]];
  sR = psiR[[iOverLap + 1]] - psiR[[iOverLap - 1]];
  xpsiL = Table[{x[[i]], psiL[[i]]}, {i, lL}];
  xpsiR = Table[{x[[i + lx - lR]], psiR[[i]]}, {i, lR}];
  ds = sL - sR;
  signn = Sign[ds];



  If[Sign[signn] == Sign[signo], eng = eng + dE];
  If[Sign[signn] != Sign[signo], dE = -dE / 2.0; eng = eng + dE];
  signo = signn];
eng




p1 = ListPlot[xpsiL, PlotStyle → Black, Joined → True];
p2 = ListPlot[xpsiR, PlotStyle → Red, Joined → True];
Show[p1, p2, PlotRange → All, AxesLabel → {"x", "ψ"}]
(*-------------------------------------------------------------------------------------------------------------------------------*)
(*-------------------------------------------------------------------------------------------------------------------------------*)
(*-------------------------------------------------------------------------------------------------------
```

```
                                                  --------------------*)
(*I solved the problem using the shotting because I couldn't
 solve using the matching at first. But then I solved using both. *)
(*The shotting method. *)

ClearAll["Global`*"]

xMax = 5.0; dx = 0.01; (*you need to increase xMax to get good approximations*)
x = Range[-xMax, xMax, dx]; lx = Length[x];
v = Table[1/2 i^2, {i, -xMax, xMax, dx}];
i0 = 0 (* central position of the well *);

nEng = 5; (* number of energy levels *)
color = {Red, Yellow, Orange, Green, Magenta};
labels = {"En0", "En1", "En2", "En3", "En4"};
engList = Table[0.0, {i, nEng}];
plot = Table[0.0, {i, nEng}];

eng = 0.01; (* first guess for E *);
psiMax = 3.0; (* top bound for psi *)

Do[
  dE = .004; (* first guess for dE *)

  (* Obtaining the sign of the initial psi RIGHT*)
  psi = Table[0.0, {i, lx}];
  psi[[i0]] = 0.0; psi[[i0 - 1]] = 0.0000000000000000000000000001;
  i = i0 + 1;
  While[Abs[psi[[i - 1]]] < psiMax && i < lx,
   psi[[i]] =
    2.0 psi[[i - 1]] - psi[[i - 2]] - 2.0 (eng - v[[i - 1]]) psi[[i - 1]] dx^2;  i++];
  psiLastR = psi[[i - 1]] ; (* Last value of psi before quitting *)

  (* Main loop for energy levels *)
  While[Abs[dE] > 0.000000000001,
   psi = Table[0.0, {i, lx}];
   psi[[i0]] = 0.0; psi[[i0 - 1]] = 0.0000000000000000000000000001;

   i = i0 + 1;
   While[Abs[psi[[i - 1]]] < psiMax && i < lx,
    psi[[i]] =
     2.0 psi[[i - 1]] - psi[[i - 2]] - 2.0 (eng - v[[i - 1]]) psi[[i - 1]] dx^2;  i++];
   psiNewR = psi[[i - 1]] ;
   If[Sign[psiNewR] == Sign[psiLastR], eng = eng + dE];
   If[Sign[psiNewR] != Sign[psiLastR], dE = -dE / 2.0; eng = eng + dE];
   psiLastR = psiNewR];
  (*-----------------------------------------------------------------------*)

  engList[[j]] = eng;
```

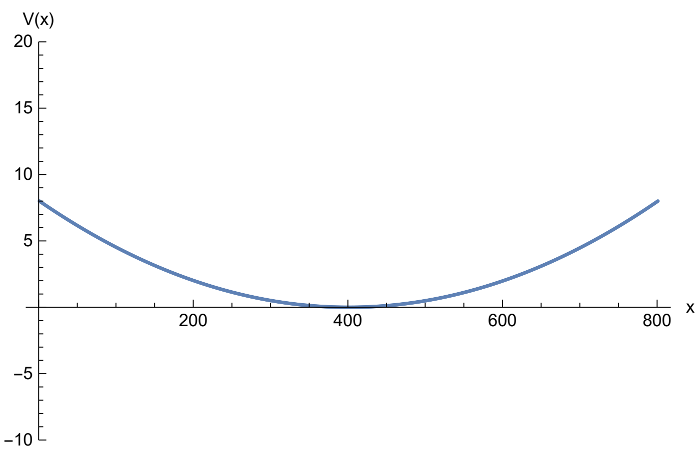
```
  eng = eng + 0.001;
  , {j, nEng}];


leg = SwatchLegend[{Red, Yellow, Orange}, {"E0", "E1", "E2"}];
englist (* shooting method *);
engExact = Table[((n - 1.0) + 1/2), {n, 5}] // StandardForm;(* Exact .. since h=m=k=1*)
ListPlot[v, Joined → True, AxesLabel → {"x", "V(x)"}, AspectRatio → 0.5, ImageSize → 600]


Print["The exact Energies for the first 5 odd levels are:\n " <> ToString [engExact] <>
  "\nestimated values from computations using the shooting method were:\n" <>
  ToString[engList]]
```

Out[∘]= 0.497186

Out[∘]=

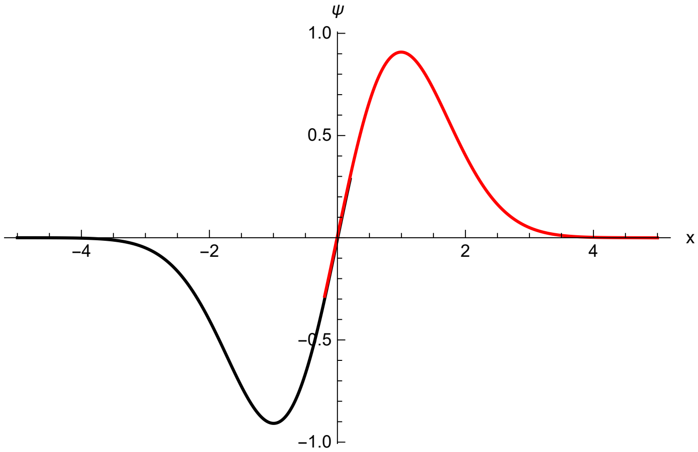


Out[∘]=

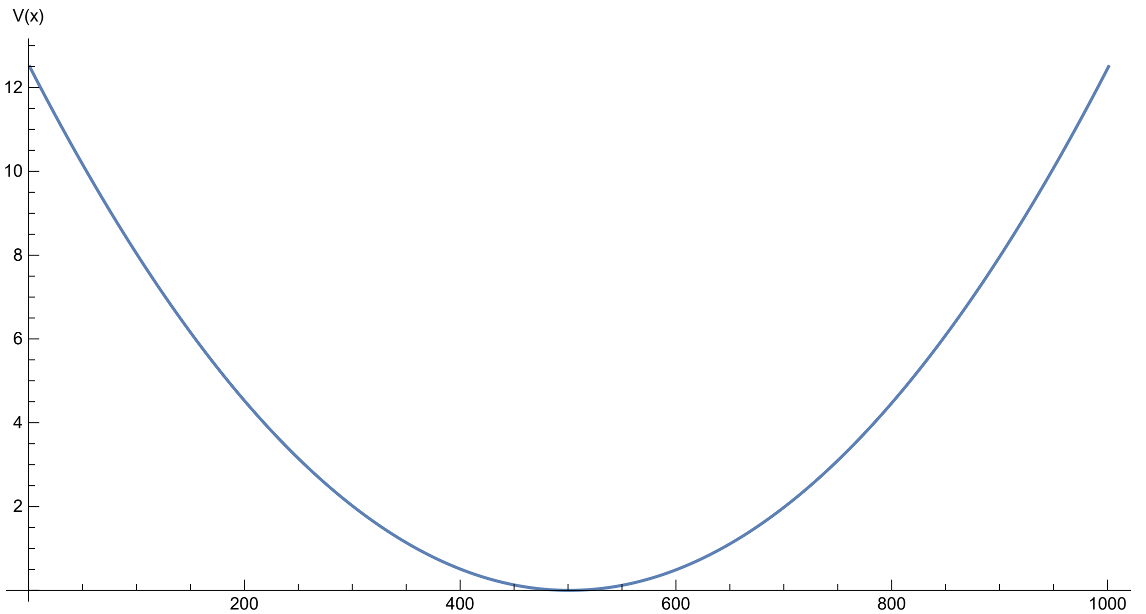


Out[∘]= 1.49435

Out[ ]=



Out[ ]=




```
The exact Energies for the first 5 odd levels are:
 {0.5, 1.5, 2.5, 3.5, 4.5}
estimated values from computations using the shooting method were:
{0.499997, 1.49998, 2.49996, 3.49992, 4.49988}
```

Problem 4: 10.7

In[ ]:=
```
(*First part for l= zero*)
ClearAll["Global`*"]
xMax = 20.0; dx = 0.05;
x = Range[0, xMax, dx]; lx = Length[x];
v = Table[-1/i, {i, 0.000000000000000000001, xMax, dx}];
(*inverse potential for the H atom*)
i0 = 1;

nEng = 3; (* number of energy levels *)
```

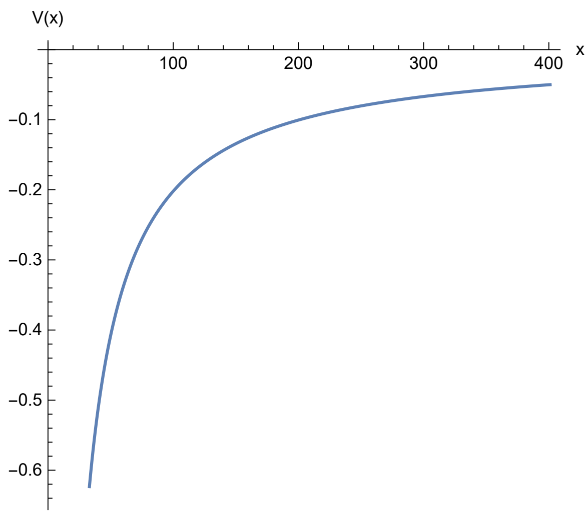
```
color = {Red, Yellow, Magenta};
labels = {"En2", "En1", "En0"};
engOddList = Table[0.0, {i, nEng}];
plot = Table[0.0, {i, nEng}];

eng = -0.001; (* first guess for E *)
psiMax = 2.0; (* top bound for psi *)

Monitor[
 Do[
  dE = -0.01; (* first guess for dE *)

  (* Obtaining the sign of the initial psi RIGHT*)
  psi = Table[0.0, {i, lx}];
  psi[[i0]] = 0.0 (*Given initial condition*); psi[[i0 + 1]] = 0.00;
  i = i0 + 2;

  (*We need to use the appropriate differential equation here for the psi calculated
   from the given radial differential equation and using the shooting method*)

  While[Abs[psi[[i - 1]]] < psiMax && i < lx,
   psi[[i]] = 2.0 psi[[i - 1]] - psi[[i - 2]] + 2 (v[[i - 1]] - eng) psi[[i - 1]] dx^2;  i++];
  psiLastR = psi[[i - 1]] ; (* Last value of psi before quitting *)

  (* Main loop for energy levels *)
  While[Abs[dE] > 0.0000000000000001,
   psi = Table[0.0, {i, lx}];
   psi[[i0]] = 0.0; psi[[i0 + 1]] = 0.0001;

   i = i0 + 2;
   While[Abs[psi[[i - 1]]] < psiMax && i < lx,
    psi[[i]] =
     (2.0 psi[[i - 1]] - psi[[i - 2]] + 2 (v[[i - 1]] - eng) psi[[i - 1]] dx^2);  i++];
   psiNewR = psi[[i - 1]] ;
   If[Sign[psiNewR] == Sign[psiLastR], eng = eng - dE];
   If[Sign[psiNewR] != Sign[psiLastR], dE = -dE / 2.0; eng = eng - dE];
   psiLastR = psiNewR];
  (*-----------------------------------------------------------------*)


  engOddList[[-j]] = eng;
  (*I used -j as an index to reverse the order since it starts to solve from the *)
  eng = eng - 0.0001;

  plot[[j]] =
   ListPlot[psi * j^1.7 300, PlotRange → All, PlotStyle → {color[[j]], PointSize → 0.005},
    (*I used a j dependent factor for the plot to adjust the relative
      sizes of each plot seperately- a kind of pseudonormalization*)
    PlotLegends → SwatchLegend[{color[[j]]}, {labels[[j]]}]]
  , {j, nEng}], ProgressIndicator[i, {j, nEng}]]
```

```
(*---------------------------------------------------------------------------*)

engOddList (* shooting method *);
engExact = Table[-1.0/(2 n^2), {n, 3}] // StandardForm;(*exact values for the hydrogen atom*)
ListPlot[v, Joined → True, AxesLabel → {"x", "V(x)"}, AspectRatio → 0.9, ImageSize → 300]
Show[plot[[1]], plot[[2]], plot[[3]], PlotRange → {-1.5, 1.5},
 AspectRatio → 0.9, ImageSize → 600, Frame → True,
 FrameLabel → {Style["X", FontSize → 15], Style["ψ", FontSize → 20]},
 PlotLabel → "3 lowest H-atom levels for (L=0)"]

Print["The exact Energies for the first 3 energy eigenvalues for (L=0) are:\n " <>
  ToString [engExact] <>
  "\nestimated values from computations using the shooting method were for (L=0):\n" <>
  ToString[engOddList]]

(*-------------------------------------------------------------------------------
                                        -----------------------------------------
                                         ----------------------------------------
                                         -------*)
(*-------------------------------------------------------------------------------
                                        -----------------------------------------
                                         ----------------------------------------
                                         -------*)
(*-------------------------------------------------------------------------------
                                        -----------------------------------------
                                         ----------------------------------------
                                         -------*)
(*-------------------------------------------------------------------------------
                                        -----------------------------------------
                                         ----------------------------------------
                                         -------*)

(*Second part for l= one*)
ClearAll["Global`*"]
xMax = 20.0; dx = 0.05;
x = Range[0, xMax, dx]; lx = Length[x];
v = Table[-1/i, {i, 0.000000000000000000001, xMax, dx}];
(*inverse potential for the H atom*)
i0 = 1;

nEng = 3; (* number of energy levels *)
color = {Red, Yellow, Magenta};
labels = {"En2", "En1", "En0"};
engOddList = Table[0.0, {i, nEng}];
plot = Table[0.0, {i, nEng}];

eng = -0.001; (* first guess for E *)
psiMax = 2.0; (* top bound for psi *)
```

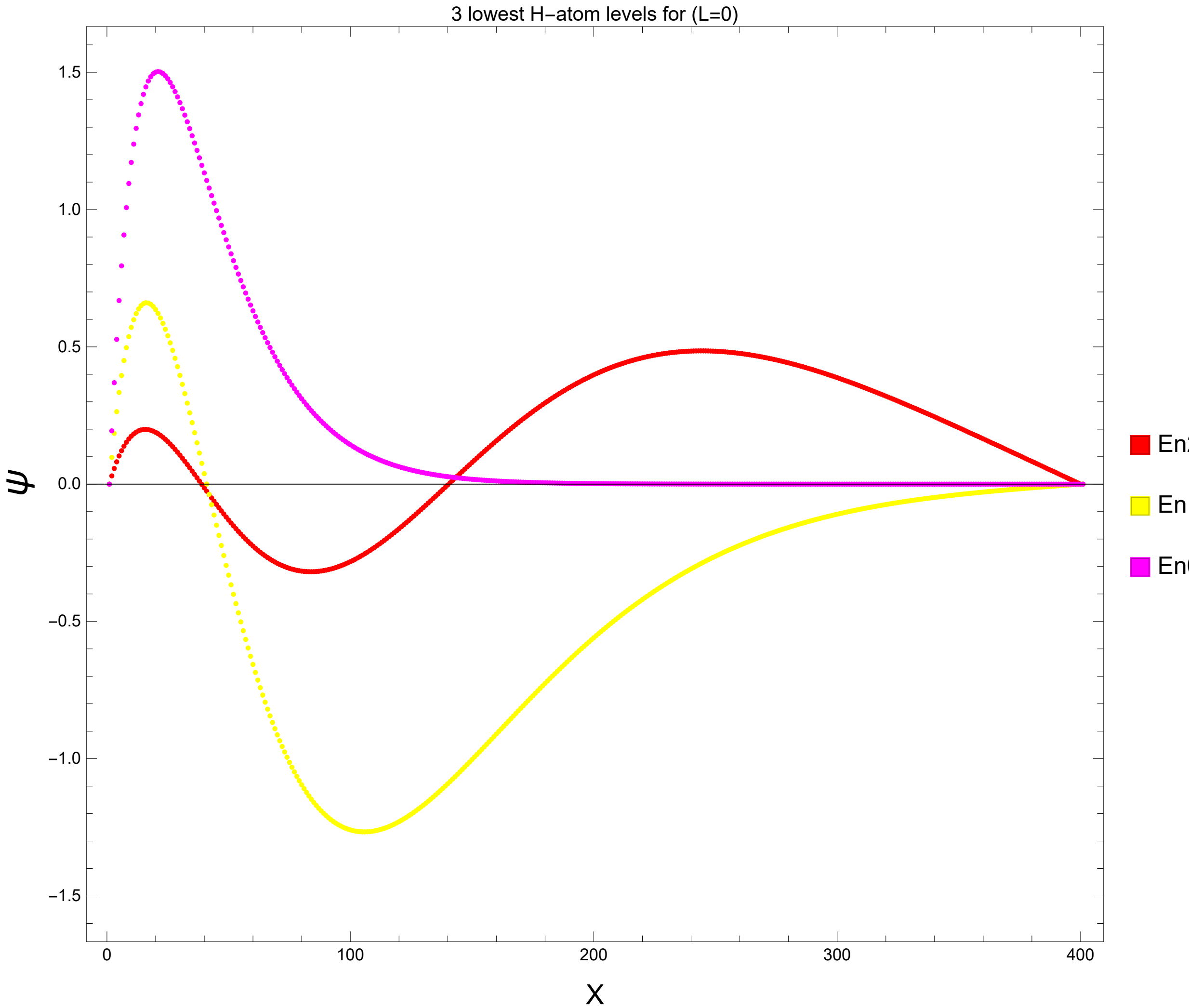
```
Monitor[
 Do[
  dE = -0.01; (* first guess for dE *)

  (* Obtaining the sign of the initial psi RIGHT*)
  psi = Table[0.0, {i, lx}];
  psi[[i0]] = 0.0 (*Given initial condition*); psi[[i0 + 1]] = 0.00;
  i = i0 + 2;

  (*We need to use the appropriate differential equation here for the psi calculated
   from the given radial differential equation and using the shooting method*)

  While[Abs[psi[[i - 1]]] < psiMax && i < lx,
   psi[[i]] = 2.0 psi[[i - 1]] - psi[[i - 2]] +
     2 (v[[i - 1]] - eng) psi[[i - 1]] dx^2 + psi[[i - 1]] * 1 * (1 + 1)/((i - 1) ^2) dx^2;  i++];
  psiLastR = psi[[i - 1]] ; (* Last value of psi before quitting *)

  (* Main loop for energy levels *)
  While[Abs[dE] > 0.0000000000000001,
   psi = Table[0.0, {i, lx}];
   psi[[i0]] = 0.0; psi[[i0 + 1]] = 0.0001;

   i = i0 + 2;
   While[Abs[psi[[i - 1]]] < psiMax && i < lx,
    psi[[i]] = (2.0 psi[[i - 1]] - psi[[i - 2]] +
       2 (v[[i - 1]] - eng) psi[[i - 1]] dx^2 + psi[[i - 1]] * 1 * (1 + 1)/((i - 1) ^2) dx^2);  i++];
   psiNewR = psi[[i - 1]] ;
   If[Sign[psiNewR] == Sign[psiLastR], eng = eng - dE];
   If[Sign[psiNewR] != Sign[psiLastR], dE = -dE / 2.0; eng = eng - dE];
   psiLastR = psiNewR];
  (*------------------------------------------------------------------*)


  engOddList[[-j]] = eng;
  (*I used -j as an index to reverse the order since it starts to solve from the *)
  eng = eng - 0.0001;

  plot[[j]] =
   ListPlot[psi * j^1.7 300, PlotRange → All, PlotStyle → {color[[j]], PointSize → 0.005},
    (*I used a j dependent factor for the plot to adjust the relative
      sizes of each plot seperately- a kind of pseudonormalization*)
    PlotLegends → SwatchLegend[{color[[j]]}, {labels[[j]]}]]
  , {j, nEng}], ProgressIndicator[i, {j, nEng}]]
(*----------------------------------------------------------------------*)
```

```
engOddList (* shooting method *);
engExact = Table[-1.0/(2 n^2), {n, 3}] // StandardForm;(*exact values for the hydrogen atom*)
ListPlot[v, Joined → True, AxesLabel → {"x", "V(x)"}, AspectRatio → 0.9, ImageSize → 300]
Show[plot[[1]], plot[[2]], plot[[3]], PlotRange → {-1.5, 1.5},
 AspectRatio → 0.9, ImageSize → 600, Frame → True,
 FrameLabel → {Style["X", FontSize → 15], Style["ψ", FontSize → 20]},
 PlotLabel → "3 lowest H-atom levels for (L=1)"]

Print[
 "The exact Energies for the first 3 energy eigenvalues  are:\n " <> ToString[engExact] <>
  "\nestimated values from computations using the shooting method were for (L=1):\n" <>
  ToString[engOddList]]
```

Out[∘]=

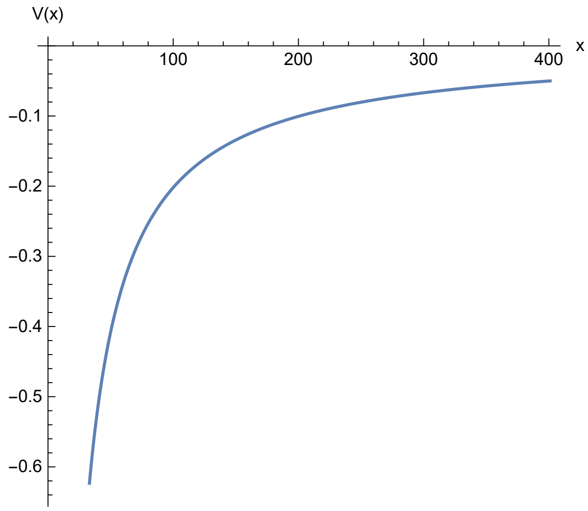


Out[•]=

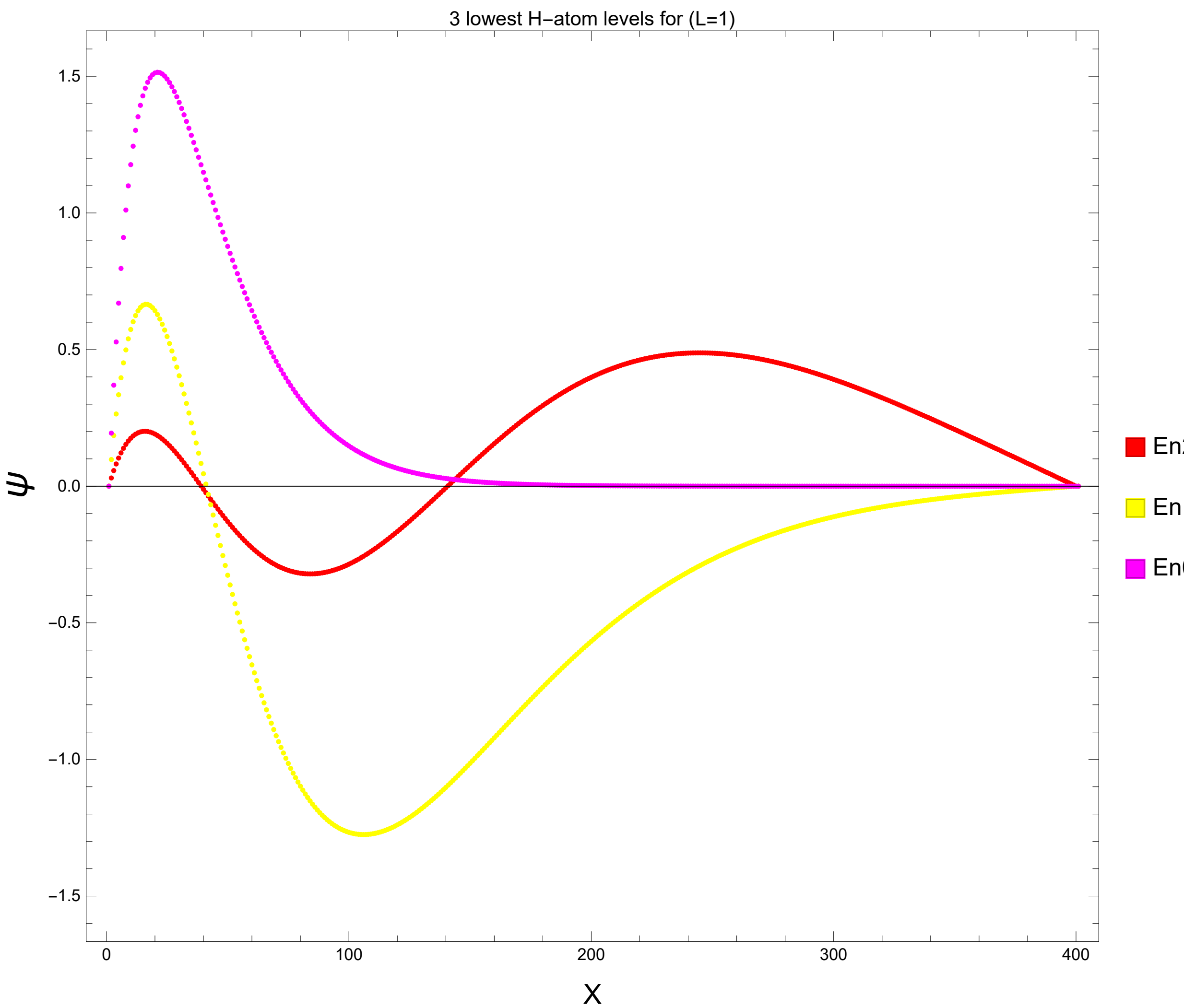


The exact Energies for the first 3 energy eigenvalues for (L=0) are:
{-0.5, -0.125, -0.0555556}
estimated values from computations using the shooting method were for (L=0):
{-0.499688, -0.124967, -0.0498172}

Out[ ]=


V(x)
x
100
200
300
400
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6

Out[ ]=


3 lowest H-atom levels for (L=1)
ψ
X
En2
En1
En0

```
The exact Energies for the first 3 energy eigenvalues  are:
 {-0.5, -0.125, -0.0555556}
estimated values from computations using the shooting method were for (L=1):
{-0.496329, -0.124539, -0.0496301}
```

Problem 5

Problem 6

Problem 7

Problem 8

Problem 9

Problem 10