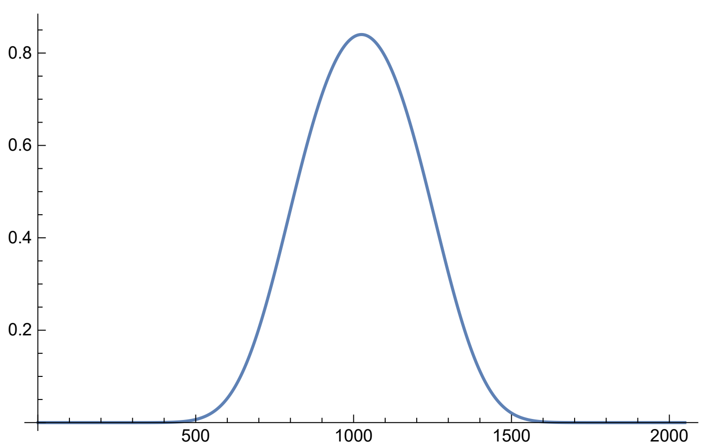
Homework 11

- Name: Eslam Muhammed Ahmed Zenhom
- ID: 201700788

Problem 1

In[ ]:=
```
(*Matrix Method*)
ClearAll["Global`*"]
dr = 2.0^-8;
r = Range[-4, 4, dr];
lr = Length[r];
pot = r^4;
d1 = -1.0/(2.0 dr^2);
d2 = 1.0/(dr^2);
hmat = Array[0 &, {lr, lr}];
hmat[[1, 1]] = pot[[1]] + d2;
hmat[[1, 2]] = d1;
hmat[[lr, lr]] = pot[[lr]] + d2;
hmat[[lr, lr - 1]] = d1;
Do[
 hmat[[i, i - 1]] = d1;
 hmat[[i, i + 1]] = d1;
 hmat[[i, i]] = pot[[i]] + d2,
 {i, 2, lr - 1}]
hmat;
psi1 = Sort[Eigensystem[hmat]][[2, -1]];
psi2 = psi1/Sqrt[psi1.psi1 dr];
ListPlot[psi2, Joined -> True]

en = Sort[Eigenvalues[hmat]];
en[[1 ;; 10]]
Print["Ground state energy:"]
Min[en] (*Ground state energy*)

(*varitional method*)
ClearAll["Global`*"]
dx = 0.05; xMin = -4; xMax = 4;
x = Range[xMin, xMax, dx]; lx = Length[x];
phi = Table[0.0, {i, lx}];
Do[
  If[x[[i]] >= -1.0 && x[[i]] <= 1.0, phi[[i]] = 0.50]
  , {i, lx}];
```

```
phi = phi / Sqrt[phi.phi dx]; (* normalization *)

ListPlot[phi]
vLJ[x_] := x^4;
pot = vLJ[x]; (* the potential *)
hmat = Array[0 &, {lx, lx}];
d2 = 1.0 / dx^2;
d1 = -0.50 / dx^2;
hmat[[1, 1]] = pot[[1]] + d2;
hmat[[1, 2]] = d1;
hmat[[lx, lx]] = pot[[lx]] + d2;
hmat[[lx, lx - 1]] = d1;
Do[
 hmat[[i, i - 1]] = d1;
 hmat[[i, i + 1]] = d1;
 hmat[[i, i]] = pot[[i]] + d2,
 {i, 2, lx - 1}]
hmat // MatrixForm;

engOld = dx phi.hmat.phi;

Do[
 nRan = RandomInteger[{1, lx}];
 phiTry = phi;
 phiTry[[nRan]] = phiTry[[nRan]] + RandomReal[{-0.2, 0.2}];
 phiTry = phiTry / Sqrt[phiTry.phiTry dx];
 engNew = dx phiTry.hmat.phiTry;
 If[engNew < engOld, phi = phiTry; engOld = engNew],
 {j, 1000000}]
engOld
ListPlot[phiTry] (* dividing by Sqrt[dx] to get the right normalization *)
```

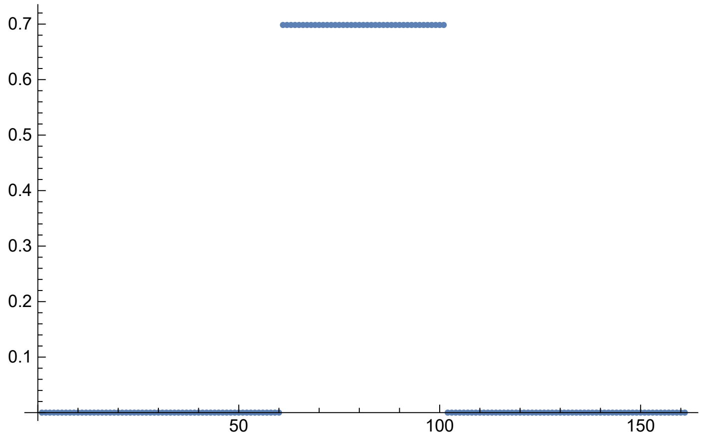
Out[ ]=


Out[ ]= {0.667985, 2.39363, 4.69676, 7.33565, 10.2442, 13.3791, 16.7115, 20.2202, 23.8892, 27.7053}

```
Ground state energy:
```

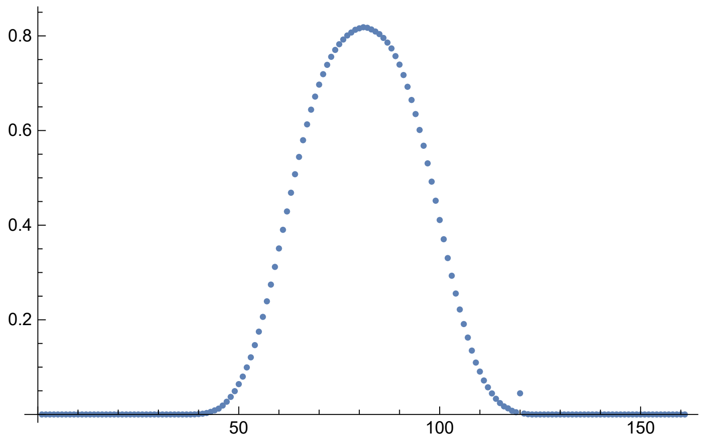
Out[ ]= 0.667985

Out[ ]=



Out[ ]= 0.678974

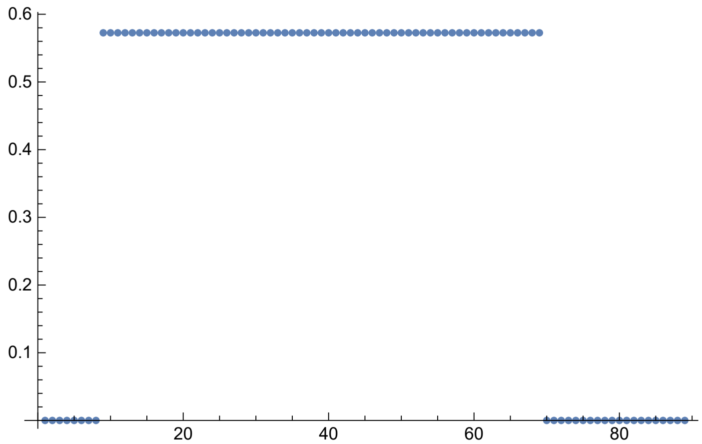
Out[ ]=



Problem 2: Fig 10.14

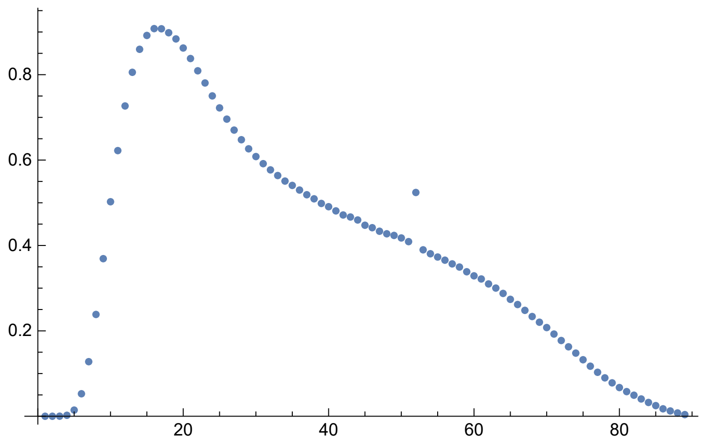
In[ ]:=
```
(*The varitional method*)

ClearAll["Global`*"]
dx = 0.05; xMin = 0.6; xMax = 5.0;
x = Range[xMin, xMax, dx]; lx = Length[x];
phi = Table[0.0, {i, lx}];
Do[
  If[x[[i]] >= 1.0 && x[[i]] <= 4.0, phi[[i]] = 0.50]
  , {i, lx}];
phi = phi/Sqrt[phi.phi dx]; (* normalization *)

ListPlot[phi]
vLJ[x_, ϵ_, σ_] := 4 ϵ ((σ/x)^12 - (σ/x)^6);
pot = vLJ[x, 8.0, 1.0]; (* Discrete potential *)
hmat = Array[0 &, {lx, lx}];
d2 = 1.0/dx^2;
d1 = -0.50/dx^2;
hmat[[1, 1]] = pot[[1]] + d2;
hmat[[1, 2]] = d1;
hmat[[lx, lx]] = pot[[lx]] + d2;
hmat[[lx, lx - 1]] = d1;
Do[
 hmat[[i, i - 1]] = d1;
 hmat[[i, i + 1]] = d1;
 hmat[[i, i]] = pot[[i]] + d2,
 {i, 2, lx - 1}]
hmat // MatrixForm;

engOld = dx phi.hmat.phi;

Do[
 nRan = RandomInteger[{1, lx}];
 phiTry = phi;
 phiTry[[nRan]] = phiTry[[nRan]] + RandomReal[{-0.2, 0.2}];
 phiTry = phiTry/Sqrt[phiTry.phiTry dx];
 engNew = dx phiTry.hmat.phiTry;
 If[engNew < engOld, phi = phiTry; engOld = engNew],
 {j, 1000000}]
engOld
ListPlot[phiTry] (* dividing by Sqrt[dx] to get the right normalization *)
```

Out[∘]=



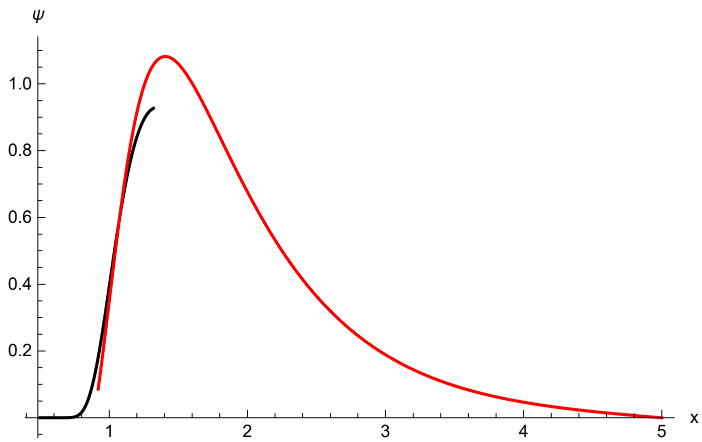
Out[∘]= -0.904465

Out[∘]=

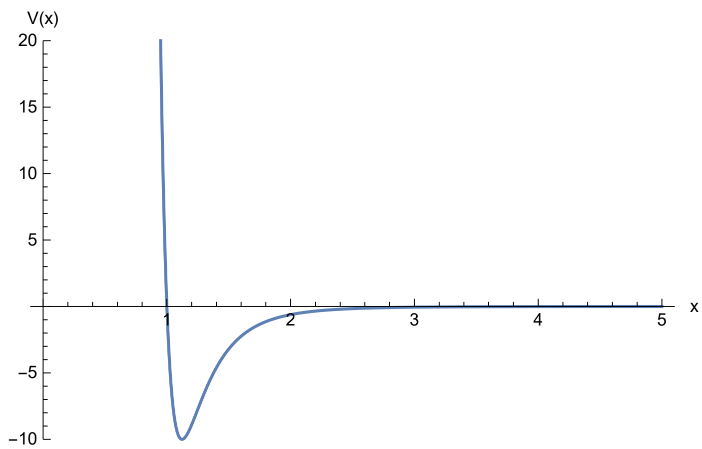


```
In[•]:= (*The matching method*)
dx = 0.01; xMin = 0.5; xMax = 5.0;
x = Range[xMin, xMax, dx]; lx = Length[x];
eng = -0.9; (* first guess for E *)

dE = .04; (* first guess for dE *)

vLJ[x_, ϵ_, σ_] := 4 ϵ ((σ/x)^12 - (σ/x)^6);
v = vLJ[x, 8.0, 1.0]; (* Discrete 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]];
xpsiL = Table[{x[[i]], psiL[[i]]}, {i, lL}];
xpsiR = Table[{x[[i + lx - lR]], psiR[[i]]}, {i, lR}];
p1 = ListPlot[xpsiL, PlotStyle → Black, Joined → True];
p2 = ListPlot[xpsiR, PlotStyle → Red, Joined → True];
Show[p1, p2, PlotRange → All, AxesLabel → {"x", "ψ"}]
Plot[vLJ[x, 10.0, 1.0], {x, 0.5, 5}, PlotRange → {{-10, 20}}, AxesLabel → {"x", "V(x)"}]
```

Out[ ]=



Out[ ]=



Problem 3

Problem 4

Problem 5

Problem 6

Problem 7

Problem 8

Problem 9

Problem 10