Homework 3I — Solution to Individual Exercises

3.016 Mathematical Methods for Materials Scientists and Engineers
S. M. Allen
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```
Clear["Global`*"]
```

Individual Exercise I3-1: (Kreyszig MCG 6.4, p. 77)

Using the matrices provided

```
A = {{1, 3, 2}, {3, 5, 0}, {2, 0, 4}}
B = {{0, 2, 1}, {−2, 0, −3}, {−1, 3, 0}}
c = {{1}, {0}, {−2}}
d = {{3}, {1}, {2}}
```

```
{{1, 3, 2}, {3, 5, 0}, {2, 0, 4}}
```

```
{{0, 2, 1}, {−2, 0, −3}, {−1, 3, 0}}
```

```
{{1}, {0}, {−2}}
```

```
{{3}, {1}, {2}}
```

Going to it:

```
B.c
```

{{−2}, {4}, {−1}}

```
% // MatrixForm
```

$$\begin{pmatrix} -2 \\ 4 \\ -1 \end{pmatrix}$$

```
Transpose[c].A.c
```

{{9}}

```
A.B.c
```

{{8}, {14}, {−8}}

```
% // MatrixForm
```

$$\begin{pmatrix} 8 \\ 14 \\ -8 \end{pmatrix}$$

```
Flatten[A.c].Flatten[Transpose[B.d]]
```

-48

```
Transpose[d].B.d
```

{{0}}

```
B.d
```

{{4}, {-12}, {0}}

As to why the result is zero, look at the eigensystem of B

```
Eigensystem[B]
```

$$\left\{\left\{i\sqrt{14}, -i\sqrt{14}, 0\right\}, \left\{\left\{\frac{3}{5}-\frac{1}{5}i\sqrt{\frac{7}{2}}, \frac{1}{5}+\frac{3}{5}i\sqrt{\frac{7}{2}}, 1\right\}, \left\{\frac{3}{5}+\frac{1}{5}i\sqrt{\frac{7}{2}}, \frac{1}{5}-\frac{3}{5}i\sqrt{\frac{7}{2}}, 1\right\}, \{-3, -1, 2\}\right\}\right\}$$

Note that the third eigenvector is equal to d and its corresponding eigenvalue is 0. Multiplication of a matrix by its eigenvector returns a parallel vector scaled in length by the corresponding eigenvalue.

Individual Exercise I3-2: (Kreyszig MCG 7.10, p. 87)

```
Clear[A, B]
```

```
A = {{3, 4}, {4, -3}}
P = {{-4, 2}, {3, -1}}
```

```
{{3, 4}, {4, -3}}
```

```
{{-4, 2}, {3, -1}}
```

```
B = Inverse[P].A.P
```

```
{{-25, 12}, {-50, 25}}
```

Note that by definition, B is similar to A (B was obtained from A by a similarity transformation).

```
EigA = Eigensystem[A]
EigB = Eigensystem[B]
```

```
{{-5, 5}, {{-1, 2}, {2, 1}}}
```

General::spell1 : Possible spelling error: new symbol name "EigB" is similar to existing symbol "EigA". More…

```
{{-5, 5}, {{3, 5}, {2, 5}}}
```

Obviously, the eigenvalues are the same.

```
Inverse[P].EigA[[2, 1]]
Inverse[P].EigA[[2, 2]]
```

$\left\{\frac{3}{2}, \frac{5}{2}\right\}$

{2, 5}

We see also that multiplication of Inverse[P] by an eigenvector of A yields an eigenvector of B (see Kreyszig AEM Theorem 1, p. 392).

Individual Exercise I3-3: (Kreyszig MCG 7.12, p. 87)

```
Clear[A]
```

Define the matrix A by

```
A = {{5, 4}, {1, 2}}
```

{{5, 4}, {1, 2}}

```
EiVecA = Eigenvectors[A]
```

{{4, 1}, {−1, 1}}

Make a square matrix of eigenvectors, each eigenvector a column of the matrix.

```
X = Transpose[EiVecA]
```

```
{{4, -1}, {1, 1}}
```

```
DMatrix = Inverse[X].A.X
```

```
{{6, 0}, {0, 1}}
```

```
Eigenvalues[A]
```

```
{6, 1}
```

Homework 3G — Solution to Group Exercises

3.016 Mathematical Methods for Materials Scientists and Engineers
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```
Clear["Global`*"]
```

Homework 3G — Solution to Group Exercises

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```
Clear["Global`*"]
```

Group Exercise G3-1: Edge Dislocation

1.

Enter the stress matrix in cartesian coordinates; use Replace to convert to Polar form.

$$\sigma_{xx} = \frac{G\,b}{2\,\pi\,(1-\nu)}\;\frac{-y\,(3\,x^2+y^2)}{(x^2+y^2)^2};$$
$$\sigma_{xy} = \frac{G\,b}{2\,\pi\,(1-\nu)}\;\frac{x\,(x^2-y^2)}{(x^2+y^2)^2};$$
$$\sigma_{yx} = \frac{G\,b}{2\,\pi\,(1-\nu)}\;\frac{x\,(x^2-y^2)}{(x^2+y^2)^2};$$
$$\sigma_{yy} = \frac{G\,b}{2\,\pi\,(1-\nu)}\;\frac{y\,(x^2-y^2)}{(x^2+y^2)^2};$$

SigMatCart = $\{\{\sigma_{xx}, \sigma_{xy}\}, \{\sigma_{yx}, \sigma_{yy}\}\}$;
MatrixForm[%]

$$\begin{pmatrix} -\frac{b\,G\,y\,(3\,x^2+y^2)}{2\,\pi\,(x^2+y^2)^2\,(1-\nu)} & \frac{b\,G\,x\,(x^2-y^2)}{2\,\pi\,(x^2+y^2)^2\,(1-\nu)} \\ \frac{b\,G\,x\,(x^2-y^2)}{2\,\pi\,(x^2+y^2)^2\,(1-\nu)} & \frac{b\,G\,y\,(x^2-y^2)}{2\,\pi\,(x^2+y^2)^2\,(1-\nu)} \end{pmatrix}$$

$\sigma_{rr} = \sigma_{xx}$ /. {x → r Sin[θ], y → r Cos[θ]};
$\sigma_{r\theta} = \sigma_{xy}$ /. {x → r Sin[θ], y → r Cos[θ]};
$\sigma_{\theta r} = \sigma_{yx}$ /. {x → r Sin[θ], y → r Cos[θ]};
$\sigma_{\theta\theta} = \sigma_{yy}$ /. {x → r Sin[θ], y → r Cos[θ]};

General::spell1 :
Possible spelling error: new symbol name "θr" is similar to existing symbol "θ". More…

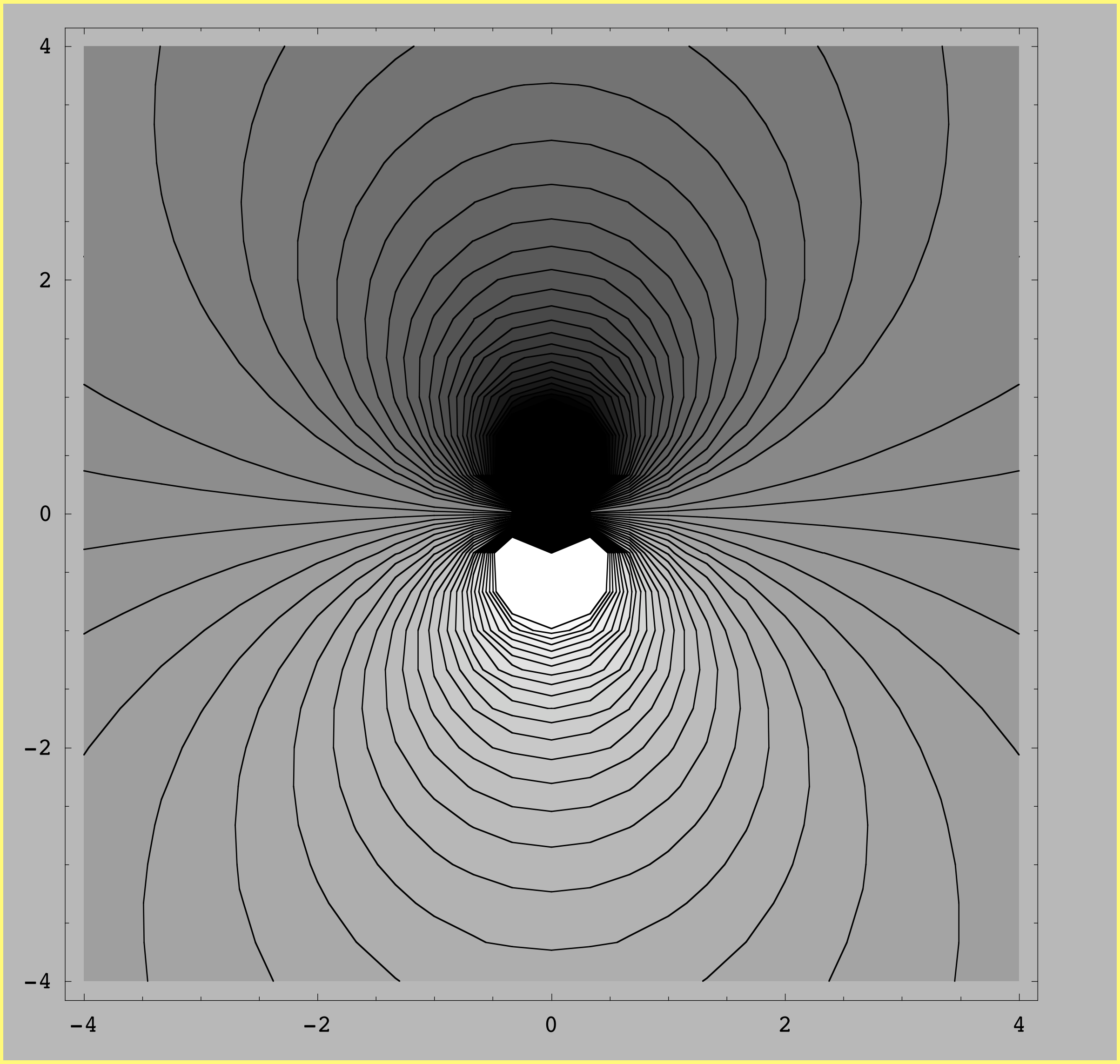
```
SigMatPolar = {{σrr, σrθ}, {σθr, σθθ}};
MatrixForm[%]
```

$$\begin{pmatrix} -\frac{b\,G\,r\,\mathrm{Cos}[\theta]\,(r^2\,\mathrm{Cos}[\theta]^2+3\,r^2\,\mathrm{Sin}[\theta]^2)}{2\,\pi\,(1-\nu)\,(r^2\,\mathrm{Cos}[\theta]^2+r^2\,\mathrm{Sin}[\theta]^2)^2} & \frac{b\,G\,r\,\mathrm{Sin}[\theta]\,(-r^2\,\mathrm{Cos}[\theta]^2+r^2\,\mathrm{Sin}}{2\,\pi\,(1-\nu)\,(r^2\,\mathrm{Cos}[\theta]^2+r^2\,\mathrm{Sin}[\theta]} \\ \frac{b\,G\,r\,\mathrm{Sin}[\theta]\,(-r^2\,\mathrm{Cos}[\theta]^2+r^2\,\mathrm{Sin}[\theta]^2)}{2\,\pi\,(1-\nu)\,(r^2\,\mathrm{Cos}[\theta]^2+r^2\,\mathrm{Sin}[\theta]^2)^2} & \frac{b\,G\,r\,\mathrm{Cos}[\theta]\,(-r^2\,\mathrm{Cos}[\theta]^2+r^2\,\mathrm{Sir}}{2\,\pi\,(1-\nu)\,(r^2\,\mathrm{Cos}[\theta]^2+r^2\,\mathrm{Sin}[\theta]} \end{pmatrix}$$

2.

$$\mathrm{HydroPress}[x\_, y\_] := \frac{2}{3}\,(\sigma_{xx} + \sigma_{yy})$$

```
ContourPlot[HydroPress[x, y] /. {G -> 1, b -> 1, ν -> 1 / 3},
  {x, -4, 4}, {y, -4, 4}, Contours → 50]
```



- ContourGraphics -

■ **3.**

Principal axes are given by eigenvectors of the stress matrix

```
evs = Eigenvectors[SigMatCart]
```

$$\left\{\left\{-\frac{-x+y}{x+y},\,1\right\},\,\left\{-\frac{x+y}{x-y},\,1\right\}\right\}$$

The orientation of principal axes can be illustrated by plotting the first eigenvector(normalized) as a function of position using PlotVectorField in the Graphics package:

```
NormEV1[x_, y_] :=
  FullSimplify[evs[[1]] / Sqrt[evs[[1, 1]]^2 + evs[[1, 2]]^2],
    Assumptions → {x ∈ Reals, y ∈ Reals}]
```

```
<< Graphics`PlotField`
```

```
PlotVectorField[NormEV1[x, y], {x, −4, 4}, {y, −4, 4}]
```

Power::infy : Infinite expression $\frac{1}{0}$ *encountered. More…*

Power::infy : Infinite expression $\frac{1}{0}$ *encountered. More…*

Power::infy : Infinite expression $\frac{1}{0}$ *encountered. More…*

General::stop : Further output of Power::infy will be suppressed during this calculation. More…

∞::indet : Indeterminate expression 0 ComplexInfinity encountered. More…

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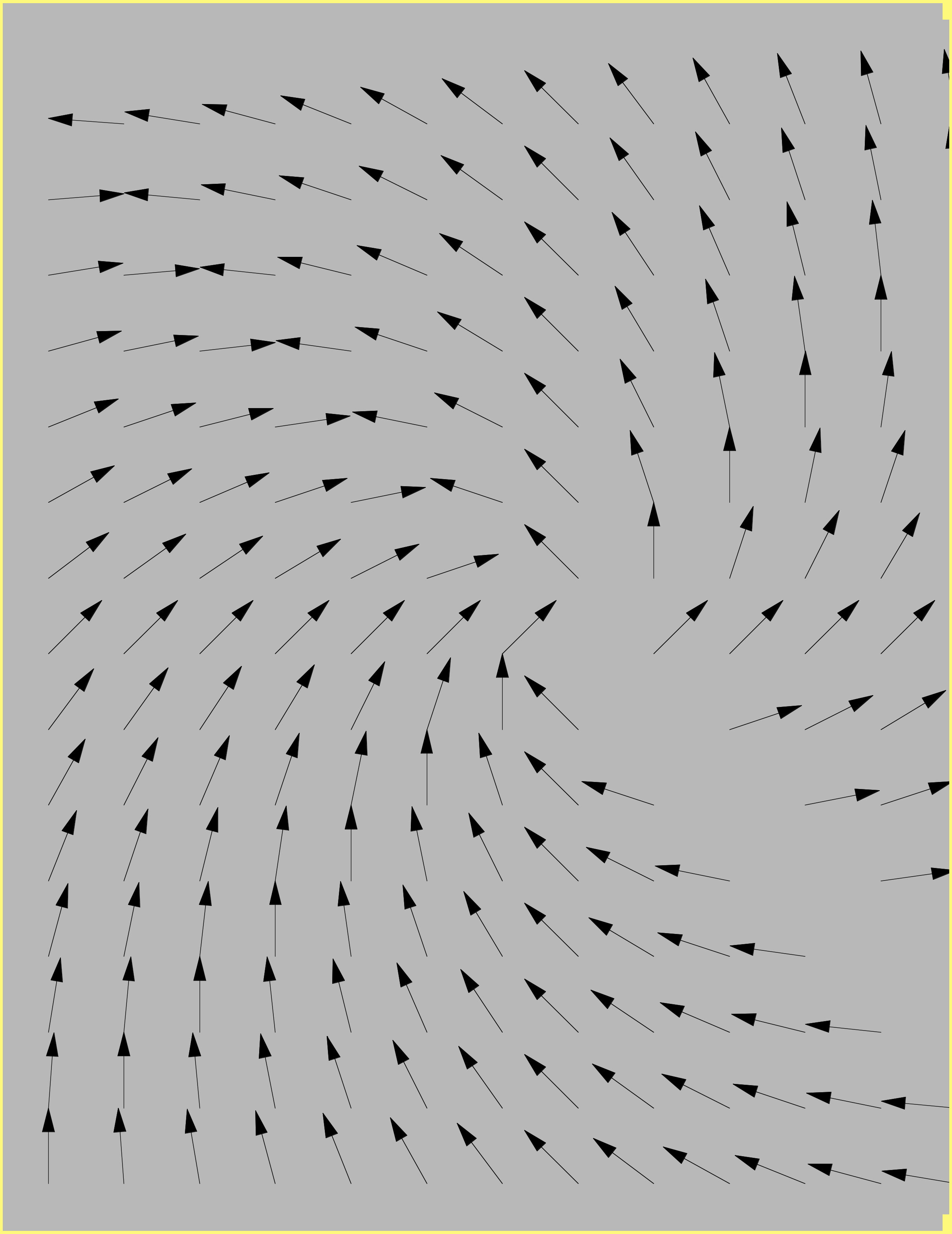
∞::indet : Indeterminate expression 0 ComplexInfinity encountered. More…

General::stop : Further output of ∞::indet will be suppressed during this calculation. More…



- Graphics -

Note that there are singularities along the line x = -y, but *Mathematica* will continue and make the remainder of the plot anyway...

Power::infy : Infinite expression $\frac{1}{0}$ encountered. More…

Power::infy : Infinite expression $\frac{1}{0}$ encountered. More…

Power::infy : Infinite expression $\frac{1}{0}$ encountered. More…

General::stop : Further output of Power::infy will be suppressed during this calculation. More…

∞::indet : Indeterminate expression 0 ComplexInfinity encountered. More…

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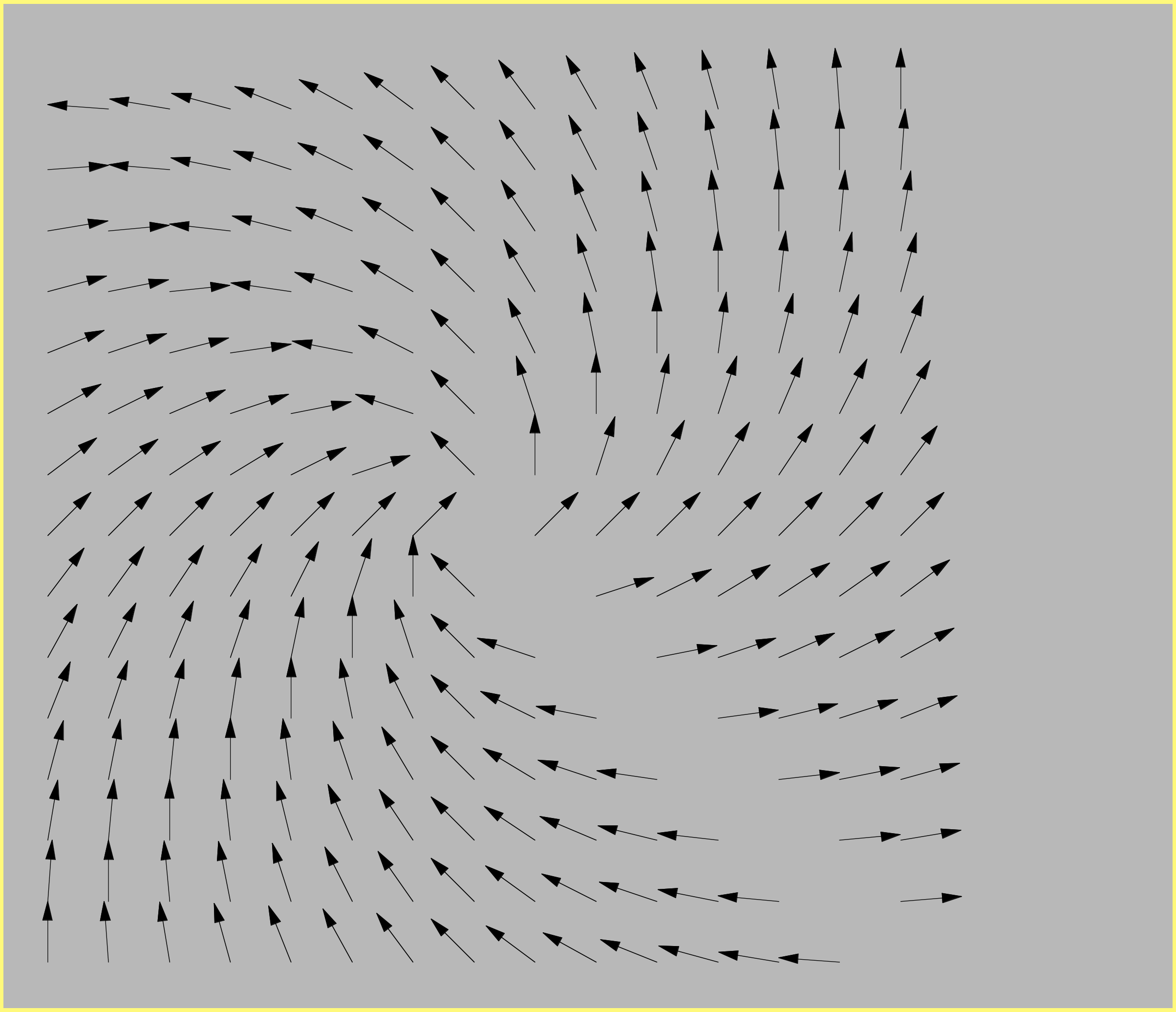
General::stop : Further output of ∞::indet will be suppressed during this calculation. More…



- Graphics -

Note how the vectors point toward each other along x = -y in the second quadrant, and away from each other along x = -y in the fourth quadrant.

■ 4.

From page 61 of the class notes (Lecture 10), it is seen that the maximum shear stress is equal to the *radius* of Mohr's circle and thus is 1/2 the *difference* between the eigenvalues of the stress matrix.

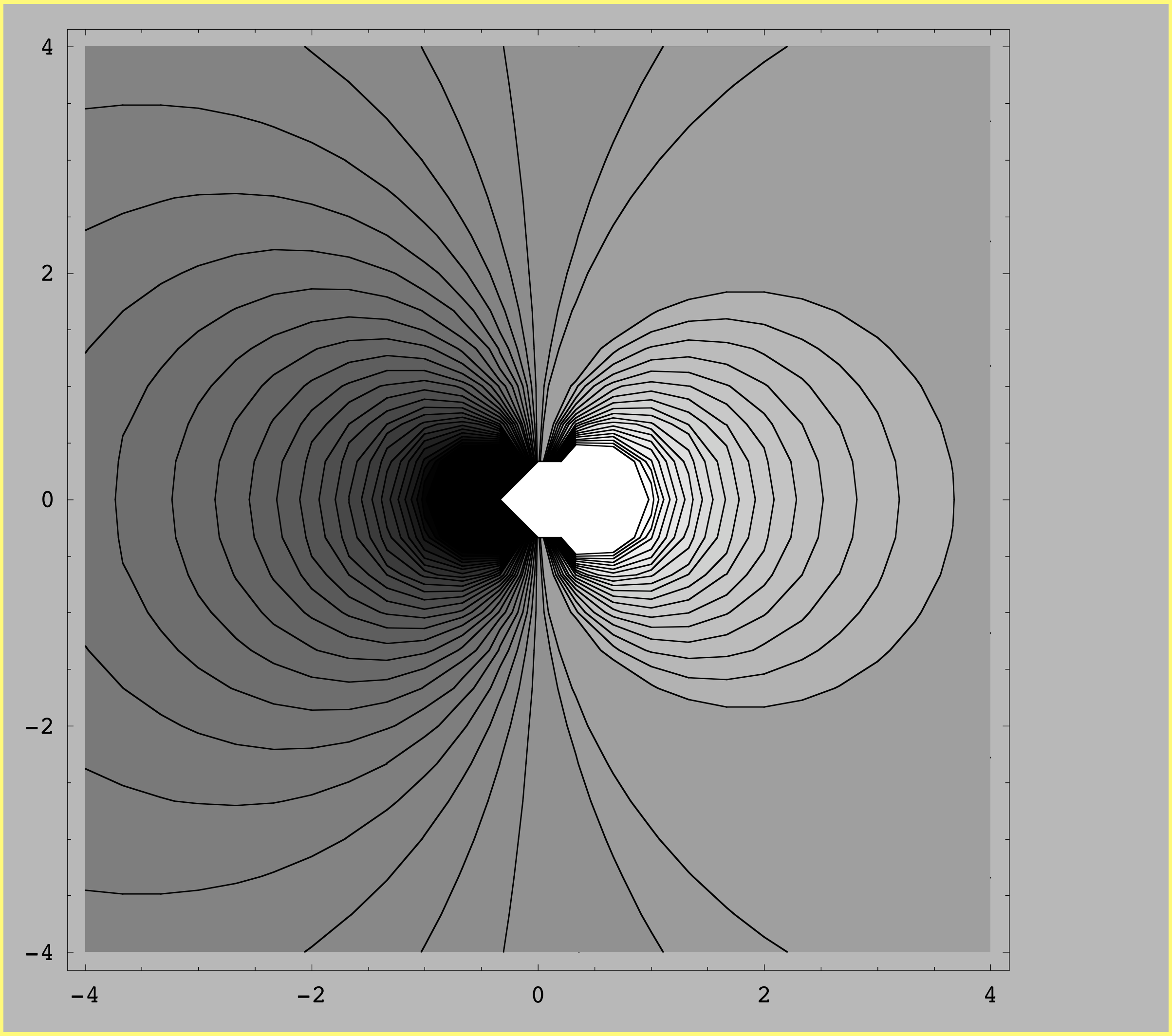
```
PrincipalStresses[x_, y_] = Eigenvalues[SigMatCart]
```

$$\left\{\frac{-b\,G\,x+b\,G\,y}{2\,\pi\,(x^2+y^2)\,(-1+\nu)},\ \frac{b\,G\,x+b\,G\,y}{2\,\pi\,(x^2+y^2)\,(-1+\nu)}\right\}$$

$$\text{MaxShear[x\_, y\_]} = \frac{1}{2}\,(\text{PrincipalStresses[x, y][[1]]} - \text{PrincipalStresses[x, y][[2]]})$$

$$\frac{1}{2}\left(\frac{-b\,G\,x+b\,G\,y}{2\,\pi\,(x^2+y^2)\,(-1+\nu)} - \frac{b\,G\,x+b\,G\,y}{2\,\pi\,(x^2+y^2)\,(-1+\nu)}\right)$$

```
ContourPlot[MaxShear[x, y] /. {G -> 1, b -> 1, ν -> 1/3},
  {x, -4, 4}, {y, -4, 4}, Contours → 50]
```



- ContourGraphics -

Note that the maximum shear stress is concentrated in the dislocation's glide plane. (See *The Structure of Materials* to learn more about dislocations and glide planes.)

Group Exercise G3-2: Entropy of Small System

Credits go to the Woolf group: Jill A. Rowehl, Jin Suk Kim, Katherine Hartman, Talia Gershon ; and to Prof. Carter, who assisted them.

Each atom can have its electron in either the n = 1 or the n = 2 states. The energy of an electron in one of these states depends on n as

$$\textbf{Energy[n\_]} := \epsilon_0 \left(1 - \frac{1}{n^2}\right)$$

- **1 and 2.**

The distinct quantum states for the three-atom system can be represented

```
States = Tuples[{1, 2}, 3]
```

```
{{1, 1, 1}, {1, 1, 2}, {1, 2, 1}, {1, 2, 2},
  {2, 1, 1}, {2, 1, 2}, {2, 2, 1}, {2, 2, 2}}
```

Make a list of energies of each of these eight states with this double summation

```
EnergyDist = {};
EnergyList =
  Do[AppendTo[EnergyDist, Sum[1 − (1 / (States[[i, j]] ^ 2)),
        {j, Length[States[[i]]]}]], {i, Length[States]}]
EnergyDist
```

General::spell1 : Possible spelling error: new symbol name "EnergyList" is similar to existing symbol "EnergyDist". More…

$$\left\{0, \frac{3}{4}, \frac{3}{4}, \frac{3}{2}, \frac{3}{4}, \frac{3}{2}, \frac{3}{2}, \frac{9}{4}\right\}$$

```
UniqueEnergies = Union[EnergyDist]
```

$$\left\{0, \frac{3}{4}, \frac{3}{2}, \frac{9}{4}\right\}$$

Here is a function that will calculate the degeneracy of energy states in a distribution:

```
EntropyVec[Elist_] :=
  Module[{uniques = Union[Elist], counts = {}},
    For[i = 1, i ≤ Length[uniques], i++,
      AppendTo[counts, {Count[Elist, uniques[[i]]]}]];
    Return[counts]]
```

```
Degeneracy = Flatten[EntropyVec[EnergyDist]]
```

{1, 3, 3, 1}

Here is the entropy of each state

```
SOverBoltzList = Log[Degeneracy]
```

```
{0, Log[3], Log[3], 0}
```

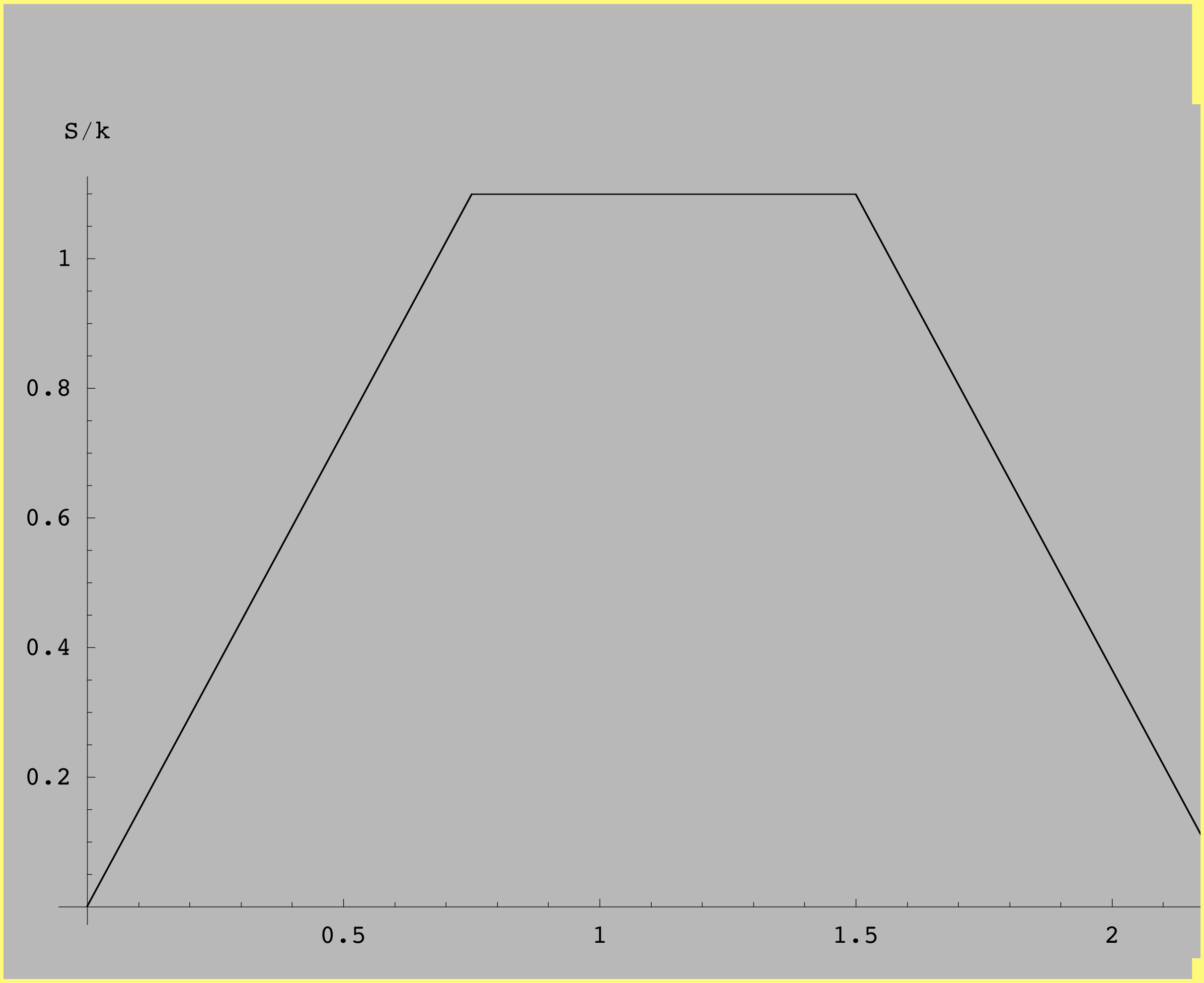
Make a function that will combine two lists and use it to make ordered pairs of {energy,entropy} which can then be plotted with ListPlot:

```
CombList[list1_, list2_] :=
  Module[{big = {}}, Do[AppendTo[big, {list1[[i]], list2[[i]]}],
     {i, Length[list1]}]; Return[big]]
```

```
SvsE = CombList[UniqueEnergies, SOverBoltzList]
```

$$\left\{\{0, 0\}, \left\{\frac{3}{4}, \text{Log}[3]\right\}, \left\{\frac{3}{2}, \text{Log}[3]\right\}, \left\{\frac{9}{4}, 0\right\}\right\}$$

```
ListPlot[SvsE, PlotJoined → True,
  AxesLabel → {"Energy", "S/k"}]
```



- Graphics -

■ **3.**

Proceed as above but for atoms that can have three energy levels n = 1, 2, or 3:

```
States = Tuples[{1, 2, 3}, 3];
```

```
EnergyDist = {};
EnergyList =
  Do[AppendTo[EnergyDist, Sum[1 - (1 / (States[[i, j]] ^ 2)),
      {j, Length[States[[i]]]}]], {i, Length[States]}]
```

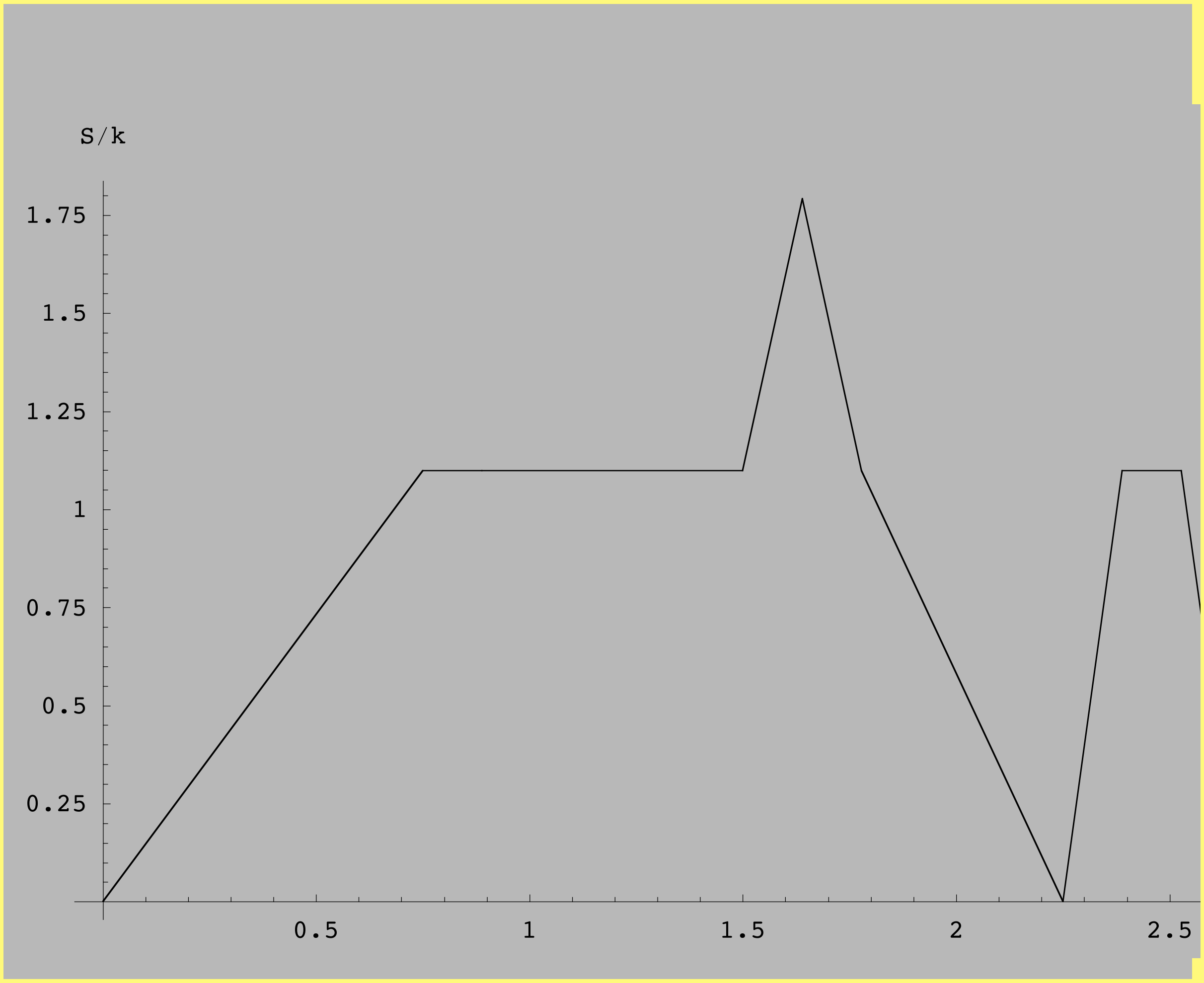
```
UniqueEnergies = Union[EnergyDist];
```

```
Degeneracy = Flatten[EntropyVec[EnergyDist]];
```

```
SOverBoltzList =  Log[Degeneracy];
```

```
SvsE = CombList[UniqueEnergies, SOverBoltzList];
```

```
ListPlot[SvsE, PlotJoined → True,
  AxesLabel → {"Energy", "S/k"}]
```



- Graphics -

■ **3.**

Proceed as above but for 5 atoms that can have three energy levels n = 1, 2, 3:

```
States = Tuples[{1, 2, 3}, 5];
```

```
EnergyDist = {};
EnergyList =
  Do[AppendTo[EnergyDist, Sum[1 - (1 / (States[[i, j]] ^ 2)),
        {j, Length[States[[i]]]}]], {i, Length[States]}]
```

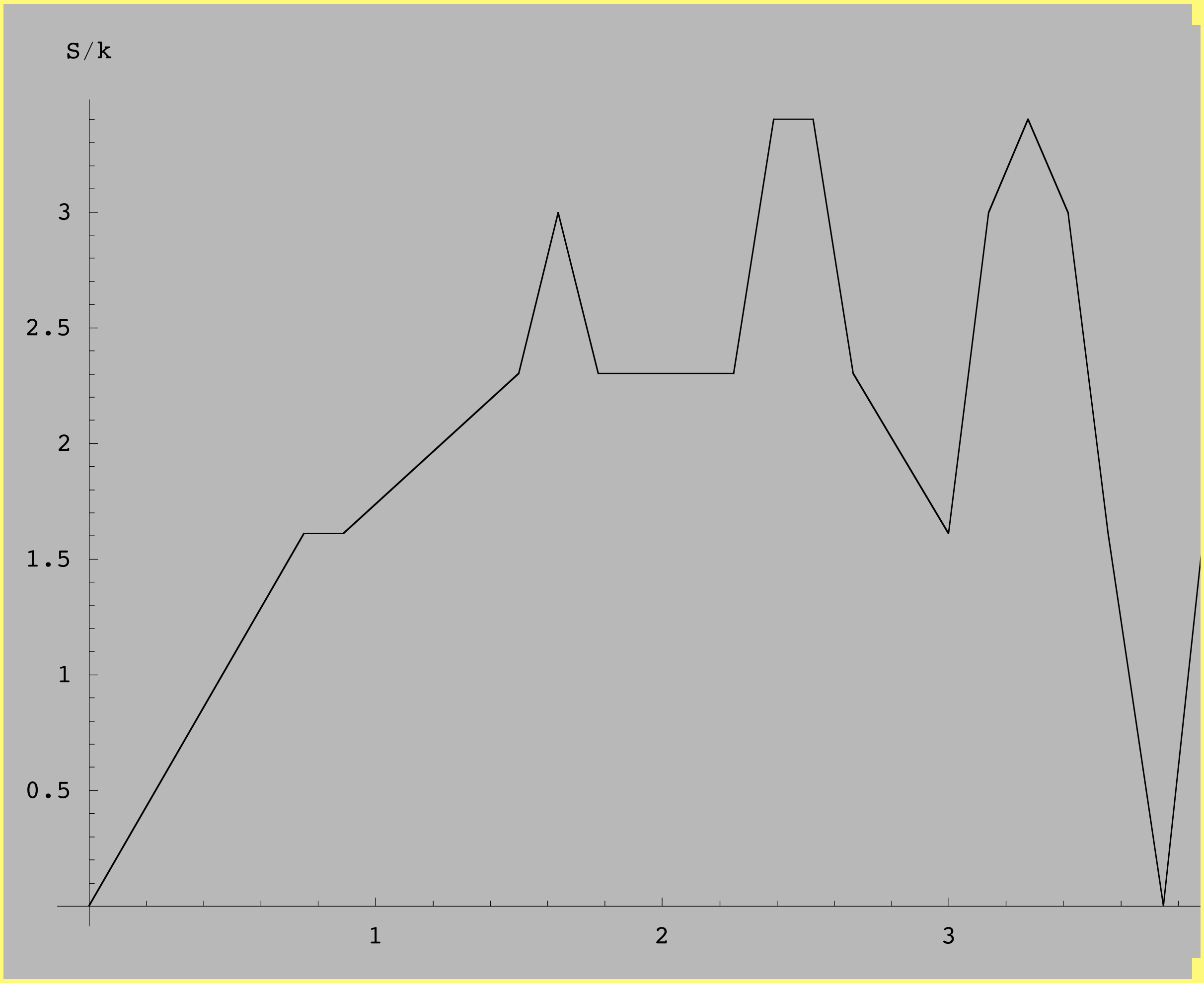
```
UniqueEnergies = Union[EnergyDist];
```

```
Degeneracy = Flatten[EntropyVec[EnergyDist]];
```

```
SOverBoltzList =  Log[Degeneracy];
```

```
SvsE = CombList[UniqueEnergies, SOverBoltzList];
```

**ListPlot[SvsE, PlotJoined → True,
AxesLabel → {"Energy", "S/k"}]**



- Graphics -

4 (Extra Credit).

Because dU = T dS - P dV, for fixed volume $(dS/dU)_V = 1/T$ and the slope of the plots above of S/k vs. Energy should be positive. Lack of accounting for high-energy states underestimates the entropy and at high temperatures S/k necessarily goes through a maximum and then falls to zero. The maximum in S/k would correspond to infinite temperature, and beyond the maximum would correspond to negative temperatures. This is unphysical.

Group Exercise G3-1: Hamiltonian

solution by WCC

Background Material

Here is the free electron Hamiltonian

$$\text{Ham[phi\_]} := \frac{-\hbar^2}{2\,m}\,\text{D[phi, \{x, 2\}]}$$

Normalize x with the characteristic distance L, and define the normalized Hamiltonian operator as

HamNorm = $\frac{H}{\frac{-\hbar^2}{2\,m\,L^2}}$ **and z = x/L**

```
HamNorm[phi_] := -D[phi, {z, 2}]
```

Define the approximating basis functions; the Hamiltonian matrix elements, and the normalizing elements

```
phi[i_] := z^i (1 - z)^i
```

```
H[i_, j_] := Evaluate[ Integrate[
      phi[i] HamNorm[phi[j]], {z, 0, 1}, Assumptions ->
        i ∈ Integers && j ∈ Integers && i > 1 && j > 1]]
```

```
F[i_, j_] :=
  Evaluate[ Integrate[phi[i] phi[j], {z, 0, 1}, Assumptions ->
        i ∈ Integers && j ∈ Integers && i > 1 && j > 1]]
```

Part 1

```
Simplify[H[i, j], Assumptions ->
    i ∈ Integers && j ∈ Integers && i > 1 && j > 1]
```

$$-\left(2^{-1-2i-2j}\, j \left(2^{1+2i+2j}(-1+j)\,\mathrm{Gamma}[-1+i+j]\,\mathrm{Gamma}[2(1+i+j)]\,\mathrm{Gamma}\left[\frac{3}{2}+i+j\right]\mathrm{Gamma}[2+i+j]\,\mathrm{Hypergeometric2F1}[-1+i+j, 3, 1+2i+2j, 1] + \mathrm{Gamma}[1+2i+2j]\left(4\left(4^{i+j}-2^{1+2i+2j}\, j\right)\mathrm{Gamma}[i+j]\,\mathrm{Gamma}\left[\frac{3}{2}+i+j\right]\mathrm{Gamma}[2+i+j]\,\mathrm{Hypergeometric2F1}[i+j, 3, 2(1+i+j), 1] + (-1+2j)\sqrt{\pi}\,\mathrm{Gamma}[1+i+j]\,\mathrm{Gamma}[2(1+i+j)]\,\mathrm{Hypergeometric2F1}[1+i+j, 3, 3+2i+2j, 1]\right)\right)\right) \Big/ \left(\mathrm{Gamma}[2(1+i+j)]\,\mathrm{Gamma}\left[\frac{3}{2}+i+j\right]\mathrm{Gamma}[1+2i+2j]\right)$$

We see that it is not at all obvious that H[i,j] == H[j,i]
but it is plausible given the explicit values below

```
H[2, 3]
```

$$\frac{1}{210}$$

```
H[3, 2]
```

$$\frac{1}{210}$$

To see if this is symmetric, try and integrate by parts:

```
dv = HamNorm[phi[j]]
```

$$-(-1+j)\,j\,(1-z)^{j}\,z^{-2+j}+2\,j^{2}\,(1-z)^{-1+j}\,z^{-1+j}-(-1+j)\,j\,(1-z)^{-2+j}\,z^{j}$$

```
v = Integrate[dv, z,
    Assumptions -> j ∈ Integers && j > 1]
```

$$-j\,(1-2\,z)\,(-(-1+z)\,z)^{-1+j}$$

```
u = phi[i]
```

$(1-z)^i z^i$

```
du = D[phi[i], z]
```

$i (1-z)^i z^{-1+i} - i (1-z)^{-1+i} z^i$

```
HNormNew = Simplify[(u v) /. z -> 1, Assumptions ->
      i ∈ Integers && j ∈ Integers && i > 1 && j > 1] -
   Simplify[(u v) /. z -> 0, Assumptions ->
      i ∈ Integers && j ∈ Integers && i > 1 && j > 1] -
   Integrate[v du, {z, 0, 1}, Assumptions ->
      i ∈ Integers && j ∈ Integers && i > 1 && j > 1]
```

```
i j (Beta[1, -1 + i + j, 1 + i + j] -
    2 Beta[1, i + j, 1 + i + j] + Beta[1, 1 + i + j,
      -1 + i + j] - 2 Beta[1, 1 + i + j, i + j])
```

Which is obviously symmetric with respect to interchange of i and j.

Test for consistency with above result

```
HNormNew /. {i -> 3, j -> 2}
HNormNew /. {j -> 2,  i ->  3}
```

$$\frac{1}{210}$$

$$\frac{1}{210}$$

Part 2

Write a function to calculate E(c1,c2,... cn)

```
Eform[approxlevel_Integer]  :=
  Sum[c[index1] c[index2] HNormNew /.
        {i -> index1, j -> index2},
      {index1, approxlevel}, {index2, approxlevel}] /
    Sum[c[index1] c[index2] F[index1, index2],
      {index1, approxlevel}, {index2, approxlevel}]
```

```
Eform[2]
```

$$\frac{\frac{c[1]^2}{3} + \frac{2}{15}\, c[1]\, c[2] + \frac{2\, c[2]^2}{105}}{\frac{c[1]^2}{30} + \frac{1}{70}\, c[1]\, c[2] + \frac{c[2]^2}{630}}$$

Find the minimum

- **The hard way:**

```
eqs[M_] := Table[D[Eform[M], c[k]] == 0, {k, M}]
vars[M_] := Table[c[k], {k, M}]
```

General::spell1 :
Possible spelling error: new symbol name "vars" is similar to existing symbol "var". More…

```
eqs[2]
```

$$\left\{\frac{\frac{2\,c[1]}{3}+\frac{2\,c[2]}{15}}{\frac{c[1]^2}{30}+\frac{1}{70}\,c[1]\,c[2]+\frac{c[2]^2}{630}}-\frac{\left(\frac{c[1]}{15}+\frac{c[2]}{70}\right)\left(\frac{c[1]^2}{3}+\frac{2}{15}\,c[1]\,c[2]+\frac{2\,c[2]^2}{105}\right)}{\left(\frac{c[1]^2}{30}+\frac{1}{70}\,c[1]\,c[2]+\frac{c[2]^2}{630}\right)^2}==0,\right.$$

$$\left.\frac{\frac{2\,c[1]}{15}+\frac{4\,c[2]}{105}}{\frac{c[1]^2}{30}+\frac{1}{70}\,c[1]\,c[2]+\frac{c[2]^2}{630}}-\frac{\left(\frac{c[1]}{70}+\frac{c[2]}{315}\right)\left(\frac{c[1]^2}{3}+\frac{2}{15}\,c[1]\,c[2]+\frac{2\,c[2]^2}{105}\right)}{\left(\frac{c[1]^2}{30}+\frac{1}{70}\,c[1]\,c[2]+\frac{c[2]^2}{630}\right)^2}==0\right\}$$

```
Clear[sols]
sols[M_] := Solve[eqs[M], vars[M]]
```

```
sols[2]
```

Solve::svars : Equations may not give solutions for all "solve" variables. More...

$$\left\{\left\{c[1]\to\frac{1}{21}\left(7\,c[2]-\sqrt{133}\,c[2]\right)\right\},\left\{c[1]\to\frac{1}{21}\left(7\,c[2]+\sqrt{133}\,c[2]\right)\right\}\right\}$$

```
Simplify[Eform[2] /. sols[2]]
```

Solve::svars : Equations may not give solutions for all "solve" variables. More…

$$\left\{\frac{28\left(-95+8\sqrt{133}\right)}{-266+23\sqrt{133}}, \frac{28\left(95+8\sqrt{133}\right)}{266+23\sqrt{133}}\right\}$$

- **The medium way:**

```
solsmed[M_] := Minimize[Eform[M], vars[M]]
```

```
solsmed[2]
```

$$\left\{4\left(14-\sqrt{133}\right), \left\{c[1]\to -1, c[2]\to \frac{1}{4}\left(7-\sqrt{133}\right)\right\}\right\}$$

- **Hmm, are these two results the same?**

$$\text{FullSimplify}\left[\frac{28\left(95+8\sqrt{133}\right)}{266+23\sqrt{133}}\right]$$

$$56-4\sqrt{133}$$

- **Yes... And now the easy way**

```
solseasy[M_] := NMinimize[Eform[M], vars[M]]
```

```
solseasy[2]
```

$\{9.86975, \{c[1] \to 0.238938, c[2] \to 0.27075\}\}$

The exact ground state energy is $E = \frac{-(2\pi)^2 \hbar^2}{8 m L^2}$ *which corresponds to* π^2 *in our normalized energy units, therefore we should compare* π^2 *with* $\frac{28\left(95+8\sqrt{133}\right)}{266+23\sqrt{133}}$

$$N\left[\frac{28\left(95+8\sqrt{133}\right)}{266+23\sqrt{133}}\right]$$
$$N[\pi^2]$$

9.86975

9.8696

Part 3

The equation between $E(\vec{c})$, $H(\vec{c})$, and can be rewritten as

$E(\vec{c})\ F(\vec{c}) = H(\vec{c})$

in our approximating scheme, this becomes a relationship between two quadratic forms:

$E(\vec{c})\quad \vec{c}\cdot F\cdot\vec{c} = \vec{c}\cdot H\cdot\vec{c}$

Take the gradient with respect to $\vec{c}$ and use the extremum condition $\nabla E = \vec{0}$

$E(\vec{c})\ F\cdot\vec{c} = H\cdot\vec{c}$

or as a Homogeneous equation,

$(H - E(\vec{c})\ F)\cdot\vec{c} = 0$

which has solutions if and only if $\det((H - E(\vec{c})\ F) = 0$

Part 4

- **The larger eigenvalue is the same as the the maximum above:**

```
NMaximize[Eform[2], vars[2]]
```

```
{102.13, {c[1] → −0.0809517, c[2] → 0.375061}}
```

- **it doesn't correlate to the other energy levels at all.**

Part 5

■ To make comparisons, let's divide the difference between the solutions by exact the ground state (normalized) energy π^2 and write a function that returns this ratio :

```
solsNormeasy[M_] :=
   (NMinimize[Eform[M], vars[M]][[1]] - π^2) / π^2
```

```
compareData = Table[{m, solsNormeasy[m]}, {m, 2, 20}]
```

$\{\{2, 0.0000147139\}, \{3, 3.43449\times10^{-9}\}, \{4, 2.63315\times10^{-13}\}, \{5, 2.24978\times10^{-14}\}, \{6, 4.90615\times10^{-11}\}, \{7, 1.4947\times10^{-11}\}, \{8, 3.40365\times10^{-12}\}, \{9, 1.98467\times10^{-12}\}, \{10, 1.65951\times10^{-11}\}, \{11, 2.0302\times10^{-13}\}, \{12, -3.59965\times10^{-16}\}, \{13, 9.76711\times10^{-12}\}, \{14, 4.66006\times10^{-10}\}, \{15, 3.89882\times10^{-10}\}, \{16, 3.90011\times10^{-10}\}, \{17, 9.35369\times10^{-12}\}, \{18, 7.2353\times10^{-14}\}, \{19, 1.04739\times10^{-10}\}, \{20, 8.07708\times10^{-12}\}\}$

```
<< Graphics`Graphics`
```

```
DisplayLater = DisplayFunction -> Identity;
DisplayNow = DisplayFunction -> $DisplayFunction;
```

```
p1 = LogListPlot[compareData,
     PlotStyle -> {PointSize[0.05], Hue[1]}, DisplayLater]
```

```
p2 = LogListPlot[compareData,
     PlotJoined -> True, DisplayLater]
```

Show[p1, p2, DisplayNow]

Graphics::gptn : Coordinate −15.4437 + 1.36438 ⅈ in {12, −15.4437 + 1.36438 ⅈ} is not a floating−point number. More…

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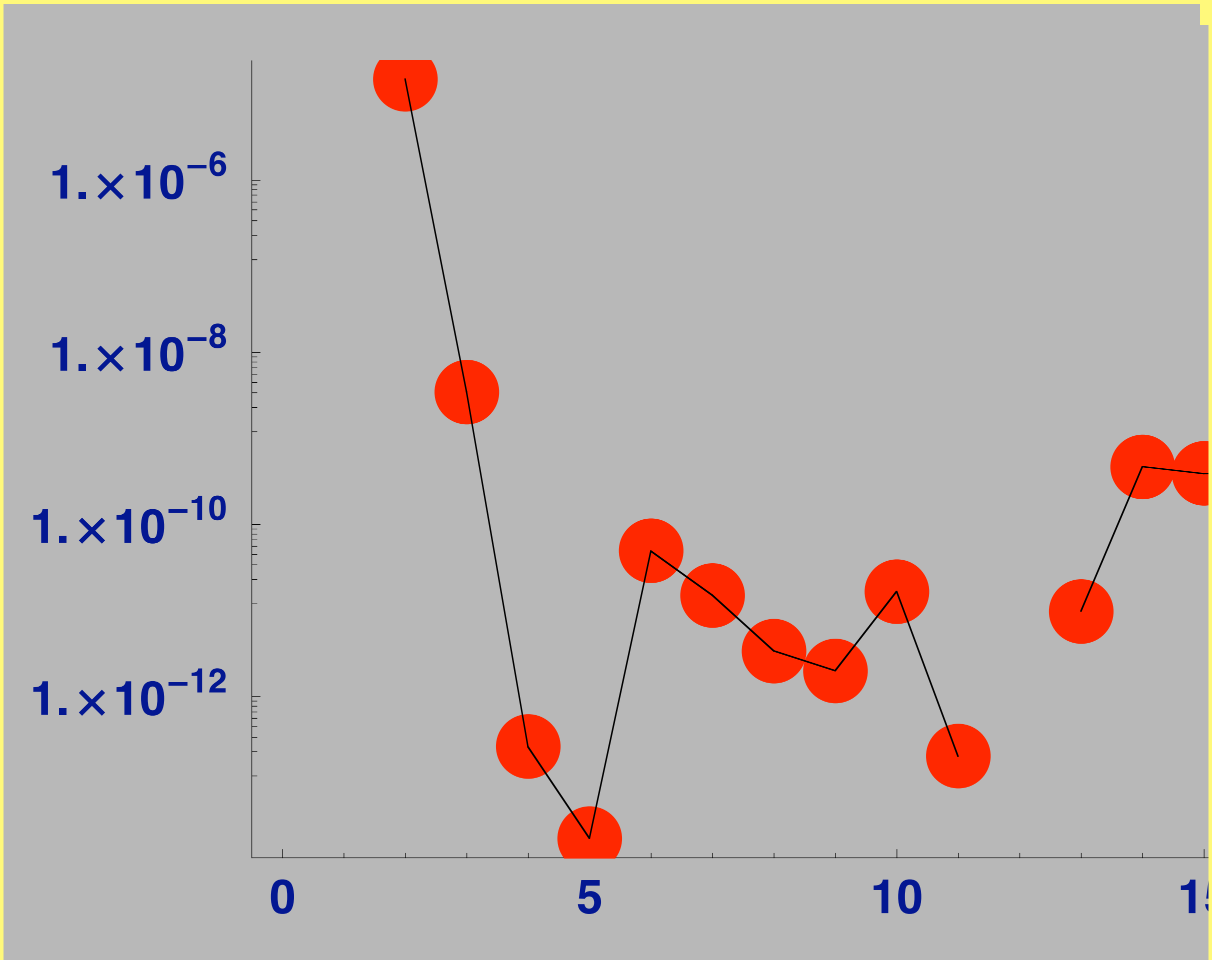

- Graphics -

- **We hit machine precision difficulties at around M=5... There is no need to go further unless we take measures to improve computation accuracy.**