Homework 26

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In[51]:=
```
SetDirectory[NotebookDirectory[]]
```
Out[51]=
```
C:\Users\carte\OneDrive\Documents\Wolfram Mathematica\360
```

Problem 1 and 2

In[52]:=
```
Import[
 "C:\\Users\\carte\\OneDrive\\Documents\\Wolfram Mathematica\\360\\hw26problems.pdf"]
```

Out[52]= {

HW 26

P1

a) $G(\varepsilon)$ has to be the octant volume divided by Δp^3. Thus

$$G_i = \frac{1}{8}\frac{4\pi}{3}\left(\frac{p_i}{\Delta p}\right)^3 = \frac{p_i^3 a^3}{6\pi^2\hbar^3} = \frac{(2m\varepsilon_i)^{3/2} V}{6\pi^2\hbar^3}$$

the momentum states and energy levels are so closely related that $\varepsilon_i \to \varepsilon$ $G_i \to G(\varepsilon)$. This is for macroscopic systems

b) $dG(\varepsilon) = g(\varepsilon)\,d\varepsilon$

$$\boxed{g(\varepsilon) = \frac{\partial G(\varepsilon)}{d\varepsilon} = \frac{d}{d\varepsilon}\frac{(2m\varepsilon_i)^{3/2} V}{6\pi^2\hbar^3} = \frac{mV}{2\pi^2\hbar^3}(2m\varepsilon)^{1/2}}$$

c) $Z_{sp} = \sum g_i e^{-\varepsilon_i/k_BT} \to \int g(\varepsilon) e^{-\varepsilon/k_BT}\,d\varepsilon$

$\xi = \varepsilon/k_BT$

$$\int g(\varepsilon) e^{-\varepsilon/k_BT}\,d\varepsilon = \int \left(mV(2m\varepsilon)^{1/2}/2\pi^2\hbar^3\right) e^{-\varepsilon/k_BT}\,d\varepsilon$$

$$= 2/\sqrt{\pi}\, V\left(mk_BT/2\pi\hbar^2\right)^{3/2}\int_0^\infty \xi^{1/2} e^{-\xi}\,d\xi$$

$$= 2/\sqrt{\pi}\, V\left(mk_BT/2\pi\hbar^2\right)^{3/2}\sqrt{\pi}/2 = V n_Q$$

,

$Z_{sp} = V n_Q$ where $n_Q = \left(\frac{m k_B T}{2\pi\hbar^2} \right)^{3/2}$

Z_{sp} is the continuous form of the single-particle partition function. We take it's integral to get rid of the Σ and then prove that $Z_{sp} = V n_Q$

P2

a) $P_i = \frac{g_i e^{-\varepsilon_i/k_B T}}{Z_{sp}} \to P(\varepsilon)\,d\varepsilon = \frac{g(\varepsilon)}{Z_{sp}(\varepsilon)} e^{-\varepsilon/k_B T}$

continuous probability that a particle has an energy between ε and $\varepsilon + d\varepsilon$

$$P(\varepsilon)d\varepsilon = \frac{g(\varepsilon) e^{-\varepsilon/k_B T}}{Z_{sp}(\varepsilon)} d\varepsilon = \left\{ \frac{mV(2m\varepsilon)^{1/2}}{2\pi^2\hbar^3} \right\} \frac{e^{-\varepsilon/k_B T}}{V n_Q(T)} d\varepsilon$$

$$\boxed{= \frac{2}{\sqrt{\pi}} \frac{\varepsilon^{1/2}}{(k_B T)^{3/2}} e^{-\varepsilon/k_B T}}$$

b) $P(v)dv = P(\varepsilon)\,d\varepsilon = P(\varepsilon(v)) \, \partial\varepsilon/\partial v \, dv$

$$= P(\varepsilon = mv^2/2)\, mv\, dv = \frac{2}{\sqrt{\pi}} \left(\frac{mv^2}{2(k_B T)^3} \right)^{1/2} e^{-mv^2/2/k_B T} mv\,dv$$

$$\boxed{= 4\pi v^2 \left(\frac{m}{2\pi k_B T} \right)^{3/2} e^{-mv^2/2k_B T}}$$

c) $P(\varepsilon)$ use $\int_0^\infty \sqrt{x}\, e^{-x} dx = \sqrt{\pi}/2$

$$\int_0^\infty P(\varepsilon)d\varepsilon = \int_0^\infty \frac{2}{\sqrt{\pi}} \frac{\varepsilon^{1/2}}{(k_B T)^{3/2}} e^{-\varepsilon/k_B T} d\varepsilon$$

$$= \frac{2}{\sqrt{\pi}} \underbrace{\left\{ \int_0^\infty \frac{\varepsilon^{1/2}}{(k_B T)^{3/2}} e^{-\varepsilon/k_B T} \right\}}_{\sqrt{\pi}/2} = \frac{2}{\sqrt{\pi}} \frac{\sqrt{\pi}}{2} = \boxed{1}$$

$P(v)$ use $\int_0^\infty x^2 e^{-x^2/2} dx = \sqrt{\pi}/\sqrt{2}$

$$\int_0^\infty P(v)dv = \int_0^\infty 4\pi v^2 \left(\frac{m}{2\pi k_B T} \right)^{3/2} e^{-mv^2/2k_B T} dv$$

$$\frac{4}{\sqrt{2}^3} = \sqrt{2} \qquad \frac{\pi}{\sqrt[2]{\pi^3}} = \frac{1}{\sqrt{\pi}} \qquad \frac{\sqrt{2}}{\sqrt{\pi}} \int_0 \underbrace{v^2 \left(\frac{m}{k_B T}\right)^{1/2} e^{-mv^2/2k_BT}}_{\sqrt{\pi}/\sqrt{2}}$$

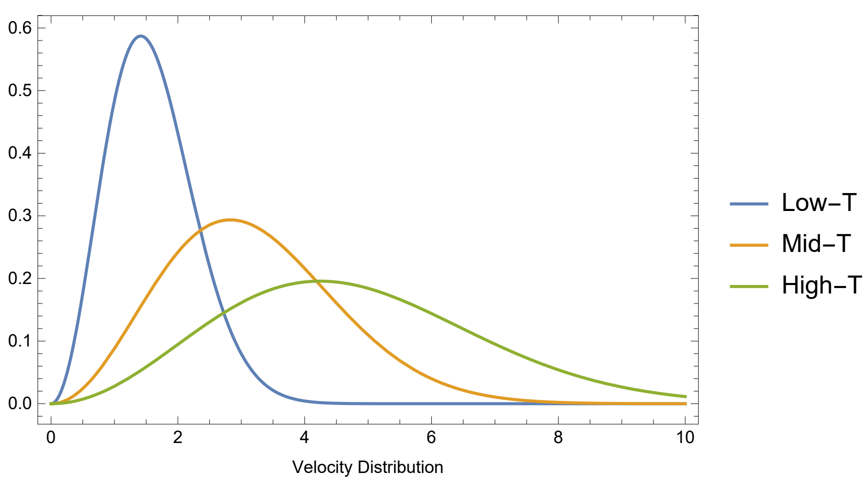
$$\frac{\sqrt{2}}{\sqrt{\pi}} \frac{\sqrt{\pi}}{\sqrt{2}} = \boxed{1}$$

Problem 3

Part A

In[1]:=
```
const = Sqrt[k * T/m];
const^-3;
const^-2;
const = 1;
Pv1 = 4 * Pi * v^2 * (1/(2 * Pi))^(3/2) * const^-3 * Exp[-v^2/2 * const^-2];
const = 2;
Pv2 = 4 * Pi * v^2 * (1/(2 * Pi))^(3/2) * const^-3 * Exp[-v^2/2 * const^-2];
const = 3;
Pv3 = 4 * Pi * v^2 * (1/(2 * Pi))^(3/2) * const^-3 * Exp[-v^2/2 * const^-2];
Plot[{Pv1, Pv2, Pv3}, {v, 0, 10}, Frame → True,
 FrameLabel → "Velocity Distribution", PlotLegends → {"Low-T", "Mid-T", "High-T"}]
```

Out[10]=



Part B

In[11]:=
$$\text{newconst} = k * \frac{T}{m};$$
$$\text{eps} = m * \frac{v^2}{2};$$
$$\text{Pv} = 4 * \text{Pi} * v^2 * \left(\frac{m}{2 * \text{Pi} * k * T}\right)^{\frac{3}{2}} * \text{Exp}\left[-m * \frac{v^2}{2 * k * T}\right];$$
$$\text{vmean} = \text{Sqrt}\left[\text{Simplify}\left[\text{Integrate}\left[v^2 * \text{Pv}, \{v, 0, \text{Infinity}\}\right]\right]\right]$$
$$\text{vmeansquared} = \text{vmean}^2$$

```
vrms = Sqrt[vmeansquared]
x = Solve[D[Pv, v] == 0, v];
vpeak = x[[3]]
```

Out[14]= $\boxed{\sqrt{3}\sqrt{\frac{k\,T}{m}} \quad \text{if} \quad \text{Re}\left[\frac{m}{k\,T}\right] > 0}$

Out[15]= $\boxed{\frac{3\,k\,T}{m} \quad \text{if} \quad \text{Re}\left[\frac{m}{k\,T}\right] > 0}$

Out[16]= $\boxed{\sqrt{3}\sqrt{\frac{k\,T}{m}} \quad \text{if} \quad \text{Re}\left[\frac{m}{k\,T}\right] > 0}$

Out[18]= $\left\{v \to \frac{\sqrt{2}\ \sqrt{k}\ \sqrt{T}}{\sqrt{m}}\right\}$

Part C

In[19]:=
$$m = \frac{(2.66 * 10^{-23})}{1000};$$
$$T = 300;$$
$$k = 1.38 * 10^{-23};$$

```
vmean
vmeansquared
vrms
vpeak
```

Out[22]= 683.313

Out[23]= 466 917.

Out[24]= 683.313

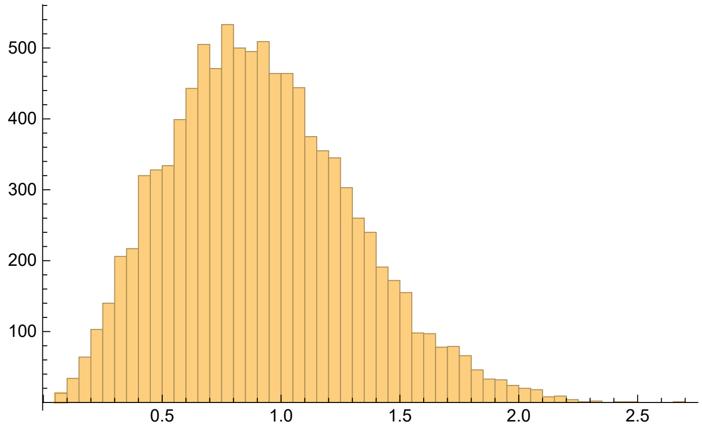
Out[25]= {v → 557.923}

Problem 4

In[26]:=
```
randomdir3D := Module[{th, z, rho}, th = RandomReal[{0, 2 Pi}];
  z = RandomReal[{-1, 1}];
  rho = Sqrt[1 - z^2];
  {rho Cos[th], rho Sin[th], z}]
collision3D[{vec1_, vec2_}] := Module[{nvec, vnorm}, nvec = randomdir3D;
  vnorm = ((vec2 - vec1).nvec) nvec;
  {vec1 + vnorm, vec2 - vnorm}]
maxbolt[{Nsize_, Nsteps_}] :=
 Module[{papavec, new1, new2, ind1, ind2, velnorm, veldist, xdata, ydata},
  papavec = Table[randomdir3D, Nsize];
  Do[
   ind1 = RandomInteger[{1, Nsize}];
   ind2 = RandomInteger[{1, Nsize}];
   {new1, new2} = collision3D[{papavec[[ind1]], papavec[[ind2]]}];
   papavec[[ind1]] = new1;
   papavec[[ind2]],
   Nsteps];
  velnorm = Norm /@ papavec;
  {xdata, ydata} = HistogramList[velnorm, 50];
  veldist = {Drop[xdata, -1] + 0.5 * (xdata[[2]] - xdata[[1]]), ydata} // Transpose;
  Return[{velnorm, veldist, Histogram[velnorm, 50]}];
 ]
take1 = maxbolt[{10000, 10}];
take2 = maxbolt[{10000, 25}];
take3 = maxbolt[{10000, 50}];
take4 = maxbolt[{10000, 100}];
take5 = maxbolt[{10000, 75}];
take6 = maxbolt[{10000, 10^6}];
take6[[3]]
gooddata = take6[[2]];
partbfit = NonlinearModelFit[gooddata, a * x1^2 * Exp[-b * x1^2], {a, b}, x1]
A = 1894.03;
B = -1.40623;
Show[Plot[A * v^2 * Exp[B * v^2], {v, 0, 5}], ListPlot[gooddata]]
b = m/(2 * k * T);
b = 1.40623;
sqrtkToverm = (2 * b)^(-1/2)
vrmsvpeakratiop = N[Sqrt[3/2]]
vpeaktrialrun = Solve[D[A * v^2 * Exp[B * v^2], v] == 0, v];
vpeak = vpeaktrialrun[[3]]
vpeak = 0.84328;
vrms = Sqrt[3] * sqrtkToverm
vrmsvpeakratioreal = vrms / vpeak
```

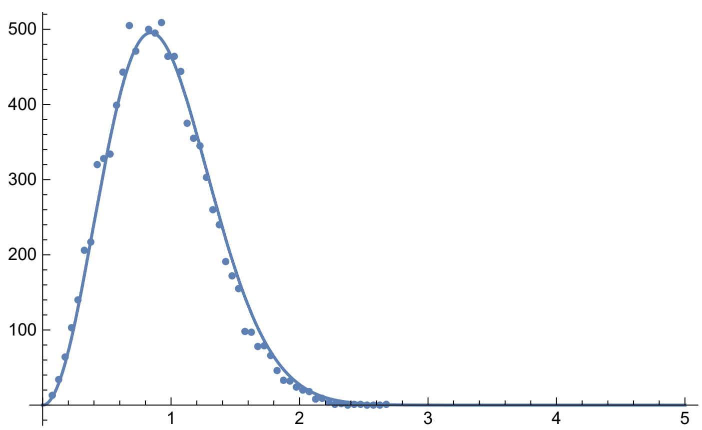
```
(* 10^6 Nsteps *)
```

Out[35]=



Out[37]= FittedModel[$2063.83\, e^{-1.4939\, x1^2}\, x1^2$]

Out[40]=



Out[43]= 0.596289

Out[44]= 1.22474

Out[46]= {v → 0.84328}

Out[48]= 1.0328

Out[49]= 1.22474