```
ClearAll["Global`*"]


(* problem 1 *********************)
(* Omega=V/6/Pi^2*(2*m*E)^(3/2)
  so d(log(Omega)/dE=1/T => (3/2)/E=1/T → E=(3/2)T *)

(* problem 2 at the end *)
(*   *************************       problem 3, ****************
  H2,D2 and HD rotations *)
ΘH2 = Θ
ΘD2 = Θ / 2
(* rotation around center of mass *)
IH2 = 2 * mN * (R / 2) ^2
IHD = mN * (2 * R / 3) ^2 + (2 * mN) * (R / 3) ^2
ID2 = (2 * mN) * 2 * (R / 2) ^2
ΘHD = Θ * IH2 / IHD
```

Out[41]= $\left\{\left\{T \to \frac{2\, hbar^2\, n^{2/3}\, \pi}{kB\, m}\right\}, \left\{T \to -\frac{2\, (-1)^{1/3}\, hbar^2\, n^{2/3}\, \pi}{kB\, m}\right\}, \left\{T \to \frac{2\, (-1)^{2/3}\, hbar^2\, n^{2/3}\, \pi}{kB\, m}\right\}\right\}$

Out[42]= Θ

Out[43]= $\frac{\Theta}{2}$

Out[44]= $\frac{mN\, R^2}{2}$

Out[45]= $\frac{2\, mN\, R^2}{3}$

Out[46]= $mN\, R^2$

Out[47]= $\frac{3\, \Theta}{4}$

In[103]:=
```
(* part b: partition functions *)
r[T_, lmax_, θ_] := Sum[(2 * L + 1) * Exp[-L * (L + 1) θ / T], {L, 0, lmax}];
rodd[T_, lmax_, θ_] :=
  Sum[((2 * L + 1) * Exp[-L * (L + 1) θ / T]) /. L → 2 k + 1, {k, 0, lmax}];
reven[T_, lmax_, θ_] := Sum[((2 * L + 1) * Exp[-L * (L + 1) θ / T]) /. L → 2 k, {k, 0, lmax}];
ZH2 = 3 * reven[T, 10, 1] + 1 * rodd[T, 10, 1]
ZD2 = 6 * reven[T, 10, 1 / 2] + 3 * rodd[T, 10, 1 / 2]
ZHD = 2 * 3 * r[T, 20, 3 / 4]
LogLogPlot[{ZH2 / T / 4, ZD2 / T / 9, ZHD / T / 6}, {T, 0.1, 10}]
```

Out[106]=
$$43 e^{-462/T} + 39 e^{-380/T} + 35 e^{-306/T} + 31 e^{-240/T} + 27 e^{-182/T} + 23 e^{-132/T} + 19 e^{-90/T} + 15 e^{-56/T} + 11 e^{-30/T} + 7 e^{-12/T} + 3 e^{-2/T} + 3 \left(1 + 41 e^{-420/T} + 37 e^{-342/T} + 33 e^{-272/T} + 29 e^{-210/T} + 25 e^{-156/T} + 21 e^{-110/T} + 17 e^{-72/T} + 13 e^{-42/T} + 9 e^{-20/T} + 5 e^{-6/T}\right)$$

Out[107]=
$$6 \left(1 + 41 e^{-210/T} + 37 e^{-171/T} + 33 e^{-136/T} + 29 e^{-105/T} + 25 e^{-78/T} + 21 e^{-55/T} + 17 e^{-36/T} + 13 e^{-21/T} + 9 e^{-10/T} + 5 e^{-3/T}\right) + 3 \left(43 e^{-231/T} + 39 e^{-190/T} + 35 e^{-153/T} + 31 e^{-120/T} + 27 e^{-91/T} + 23 e^{-66/T} + 19 e^{-45/T} + 15 e^{-28/T} + 11 e^{-15/T} + 7 e^{-6/T} + 3 e^{-1/T}\right)$$

Out[108]=
$$6 \left(1 + 41 e^{-315/T} + 39 e^{-285/T} + 37 e^{-\frac{513}{2}/T} + 35 e^{-\frac{459}{2}/T} + 33 e^{-204/T} + 31 e^{-180/T} + 29 e^{-\frac{315}{2}/T} + 27 e^{-\frac{273}{2}/T} + 25 e^{-117/T} + 23 e^{-99/T} + 21 e^{-\frac{165}{2}/T} + 19 e^{-\frac{135}{2}/T} + 17 e^{-54/T} + 15 e^{-42/T} + 13 e^{-\frac{63}{2}/T} + 11 e^{-\frac{45}{2}/T} + 9 e^{-15/T} + 7 e^{-9/T} + 5 e^{-\frac{9}{2}/T} + 3 e^{-\frac{3}{2}/T}\right)$$

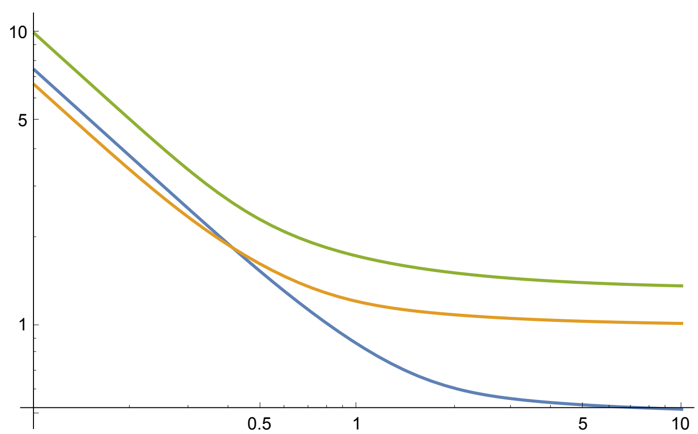
General: Exp[-4619.57] is too small to represent as a normalized machine number; precision may be lost.

General: Exp[-3799.64] is too small to represent as a normalized machine number; precision may be lost.

General: Exp[-3059.71] is too small to represent as a normalized machine number; precision may be lost.

General: Further output of General::munfl will be suppressed during this calculation.

Out[109]=



In[110]:=
```
(* let me select some T such as equal theta  and divide out degeneracy*)
ZH2 = (3. * reven[1., 5, 1] + 1 * rodd[1., 10, 1]) / 4
ZD2 = (6. * reven[1., 5, 1 / 2] + 3 * rodd[1., 10, 1 / 2]) / 9
ZHD = r[1., 10, 3 / 4]
```

Out[110]= 0.860808

Out[111]= 1.20656

Out[112]= 1.7258

In[122]:=
```
(* ********************** problem 4 *****************
   (a) from conditions it follows that
  δNH2= δND2=-(1/2)δNHD from which
    (NHD)2/NH2/ND2=fHD^2/fH2/fD2
    where each f is partition function,
consisting each of 3 factors f=Z(translational)Z(rotational)Z(vibrational)
   let us discuss each of them

   (b)
   ZHD^2/ZH2/ZD2(translational) =
  [MHD^2/MH2/MD2]^(3/2)=[3*3/2/4]^(3/2)

     T high: in classical approximation
       (sum over L → integral) it is the ratio of moments of inertia
       ZHD^2/ZH2/ZD2(rotational) =[IH2*ID2/IHD^2]
      and all three I's calculated above

      T << hbar omega → only the lowest state included,
only zero point oscillations
  ZHD^2/ZH2/ZD2(vibrational)=exp[-(2ωHD-ωH2-ωD2)*hbar/2/kB/T]
   If vibrational Hamiltonian is harmonic oscillator H=m*v^2/2+α*x^2/2,
then ω=(α/m)^(1/2). Assuming
  α is the same, only m differs (MN=nucleon mass)
  1/mH2=1/MN+1/MN; 1/mD2=1/(2*MN)+1/(2*MN); 1/mHD=1/MN+1/(2*MN)
*)
mH2 = (1 / MN + 1 / MN) ^ (-1)
mD2 = (1 / (2 * MN) + 1 / (2 * MN)) ^ (-1)
mHD = (1 / MN + 1 / (2 * MN)) ^ (-1)
(* bracket in formula above (2ωHD-ωH2-ωD2)/Sqrt[α] is *)
bracket = Assuming[MN > 0, Simplify[(2 / Sqrt[mHD] - 1 / Sqrt[mH2] - 1 / Sqrt[mD2])]]
```

Out[122]= $\frac{MN}{2}$

Out[123]= MN

Out[124]= $\frac{2\,MN}{3}$

Out[125]= $\frac{-1-\sqrt{2}+\sqrt{6}}{\sqrt{MN}}$

```
(* numerically the bracket turns out to be rather small *)
```

In[126]:= $\left(-1.-\sqrt{2.}+\sqrt{6.}\right)$

```
0.03527618041008296`
(* T-dependence is exp[-Sqrt[α/MN]*0.035/2/kB/T]
```

In[63]:=
```
(* problem 2 **************************)
ClearAll["Global`*"]
kB = 1.38064852 × 10^(-23) * m^2 * kg / s^2 / K;
hbar = 6.626176 * 10^(-34) * kg * m^2 / s;
n = 10^(21) / m^3;
mass = 87 * 1.67 * 10^(-27) * kg;
(*Solve[n == (mass*kB*T/2/Pi/hbar^2)^(3/2), T] *)
Assuming[m > 0 && kg > 0, Simplify[T = 2 hbar^2 n^(2/3) π / (kB mass)]]
```

$$T = \frac{2\, \text{hbar}^2\, n^{2/3}\, \pi}{\text{kB mass}}$$

Out[68]= 0.000137527 K