Homework 9, Problem 1:

Eq. (1): $$N(E_i) = \frac{1}{\exp(\beta E_i - \beta\mu) - 1}$$

$$= \frac{1}{\exp(\beta E_i)\,\exp(-\beta\mu) - 1}$$

$$= \frac{z}{\exp(\beta E_i) - z}$$

$z = \exp(\beta\mu)$

$$\boxed{N(E_i) = \frac{z\exp(-\beta E_i)}{1 - z\exp(-\beta E_i)}} \quad \text{Eq. (1)}$$

Eq. (2): $$\boxed{N = \sum_{i=0}^{\infty} N(E_i)} \quad \text{Eq. (2)}$$

Note: the energies of the single-particle system are labeled $E_0, E_1, E_2, \ldots$

E_j and E_i could have the same value

To get Eq. (3), we recall the expression for the geometric series:

$$\sum_{k=1}^{\infty} r^k = \frac{r}{1-r} \qquad \underbrace{\text{for } |r|<1}$$

this condition is important: convergence requires $|r|<1$!!!

Let's use Eq. (2) and plug in Eq. (1):

$$N = \sum_{i=0}^{\infty} \frac{z \exp(-\beta E_i)}{1 - z \exp(-\beta E_i)}$$

let $r_i = z \exp(-\beta E_i)$

$$= \sum_{i=0}^{\infty} \frac{r_i}{1 - r_i}$$

$$= \sum_{i=0}^{\infty} \sum_{k=1}^{\infty} (r_i)^k$$

applying the geometric series "backwards" (assumes $|r_i| < 1$)

$$\boxed{N = \sum_{i=0}^{\infty} \sum_{j=1}^{\infty} z^j \exp(-j \beta E_i)} \quad \text{Eq. (3)}$$

use j, just as the paper

for later: Eq. (3) is valid provided $|r_i| < 1$, i.e., provided

$|z \exp(-\beta E_i)| < 1$ for all i

(i.e., for all energy levels)

To obtain Eq. (4), we recognize that the energies of a single 3D harmonic oscillator with angular frequency ω are given by

$$E_{n_x n_y n_z} = (n_x + n_y + n_z)\,\hbar\omega$$

$$n_x, n_y, n_z = 0, 1, \ldots$$

note: the zero point energy is taken out (potential shifted down)

Switching the order of the sums in Eq. (3), we have

$$N = \sum_{j=1}^{\infty} z^j \underbrace{\sum_{i=0}^{\infty} \exp(-j\beta E_i)}_{\left(\sum_{n=0}^{\infty} \exp(-jn\beta\hbar\omega)\right)^3}$$

$$\boxed{N = \sum_{j=1}^{\infty} z^j \cdot \frac{1}{(1-x^j)^3}}$$ this is Eq. (4)

Eq. (4)

$$1 + x + x^2 + \ldots = \frac{1}{1-x}$$

this assumes $-1 < x < 1$ $\Rightarrow$

$$x = \exp(-\beta\hbar\omega)$$

We want to derive Eq. (6):

Start w/ Eq. (4) and rewrite:

$$N = \sum_{j=1}^{\infty} \frac{z^j}{(1-x^j)^3}$$

$$= \frac{z}{1-z} + \sum_{j=1}^{\infty} \frac{z^j}{(1-x^j)^3} \underbrace{- \frac{z}{1-z}}_{-\sum_{j=1}^{\infty} z^j}$$

these terms obviously cancel

$$= \frac{z}{1-z} + \underbrace{\sum_{j=1}^{\infty} z^j \left[\frac{1}{(1-x^j)^3} - 1 \right]}_{\text{this sum is now converging}}$$

Identifying $\frac{z}{1-z}$ as N_0, we have

$$\Rightarrow N - N_0 = \sum_{j=1}^{\infty} z^j \left[\frac{1}{(1-x^j)^3} - 1 \right]$$

Recall $x = \exp(-\beta \hbar\omega) = \exp\left(-\frac{\hbar\omega}{kT}\right)$

$$= \exp(-\tilde{\omega})$$

$$\tilde{\omega} = \frac{\hbar\omega}{kT}$$

let's look at large T limit:

$$\frac{1}{(1-e^{-j\tilde{\omega}})^3} \approx \frac{1}{(j\tilde{\omega})^3} + \frac{3}{2(j\tilde{\omega})^2} + \ldots$$

$$\Rightarrow N - N_0 \xrightarrow[\tilde{\omega} \ll 1]{} \underbrace{\sum_{j=1}^{\infty} \frac{z^j}{j^3}}_{g_3(z)} \frac{1}{\tilde{\omega}^3} + \underbrace{\sum_{j=1}^{\infty} \frac{z^j}{j^2}}_{g_2(z)} \frac{3}{2\tilde{\omega}^2} + \ldots$$

So: $\boxed{N - N_0 \approx g_3(z)\left(\frac{kT}{\hbar\omega}\right)^3 + \frac{3}{2} g_2(z)\left(\frac{kT}{\hbar\omega}\right)^2 + \ldots}$

Eq. (6) if $N_0 = \frac{z}{1-z}$

A couple of useful comments:

- The zero-point energy of the HO has been set to zero. We can always choose our energy scale in this way (shifting the potential).

- How do we know $N_0 = \frac{z}{1-z}$?

  Look at Eq. (1): Set $E_{ground} = 0$ and assume that all particles are in the ground state:

$$N_0 = \frac{z}{1-z}$$

can be rewritten:

$$N_0 = (1 + N_0) z$$

$$z = \frac{N_0}{N_0 + 1}$$

as $T \to 0$: $z \to \frac{N_0}{N_0+1}$

(less than 1)

we also know

$z \to 0 \qquad T \to \infty$

- we have worked, so far, with the discrete energy levels and carried out the sums $\rightsquigarrow$ no divergencies or bad behaviors were encountered

Homework 9, Problem 2:

Let's go back to Eq. (3):

$$N = \sum_{i=0}^{\infty} \sum_{j=1}^{\infty} z^j \exp(-j\beta E_i)$$

$$= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} z^j \exp(-j\beta E_i)$$

$$+ \underbrace{\sum_{j=1}^{\infty} z^j}_{\frac{z}{1-z} = N_0}$$

$$= N_0 + \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} z^j \exp(-j\beta E_i)$$

$$\boxed{N = N_0 + \sum_{j=1}^{\infty} z^j \underbrace{\sum_{i=1}^{\infty} \exp(-j\beta E_i)}_{\int_0^\infty \underbrace{\rho(E)}_{\text{density of states}} e^{-j\beta E}\, dE}} \quad \text{Eq. (7)}$$

For the 3D HO, we have a degeneracy of $(n+1)(n+2)/2$

The leading-order term of the degeneracy factor scales as $n^2/2$

$$\Rightarrow \quad \rho(E) = \frac{1}{2}\left(E/\hbar\omega\right)^2 \frac{1}{\hbar\omega}$$

# of states per energy interval

If we evaluate the integral, we have

$$\boxed{N - N_0 = g_3(z)\left(\frac{k_B T}{\hbar\omega}\right)^3} \qquad \text{Eq. (8)}$$

see Mathematica notebook

We now define the transition temperature by setting $N_0 = 0$ and $z = 1$

$$\Rightarrow \quad N = g_3(1)\left(\frac{k_B T_c^0}{\hbar\omega}\right)^3$$

or $$\boxed{k_B T_c^0 = \left(\frac{N}{g_3(1)}\right)^{1/3} \hbar\omega} \qquad \text{Eq. (5)}$$

Problem 4:

We need to find z : z is determined by Eq. (4)

$$\text{Eq. (4)} \rightsquigarrow \sum_{j=0}^{\infty} \frac{z^j}{\left[1-\exp\left(-\frac{\hbar\omega}{kT}\right)\right]^3} - N_{ave} = 0$$

function Nz in notebook

in our case, $N_{ave} = 100$

in our numerics, we cannot go to ∞: for $N=100$, the notebook shows that the results are approximately converged for $j_{max} = 500$

We want to find z such that Eq. (4) holds.

Since we need to calculate the sum numerically, we need to find the solution to Eq. (4) by looking at which z works → use RootFind

⇝ when using RootFind, it is always helpful to first plot the function...

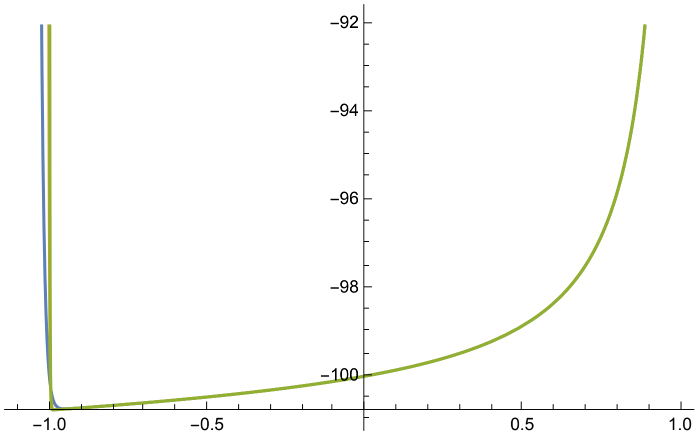
Note: T_c^0 is given in Eq. (5). If we know N_{ave}, we can calculate T_c^0 (it is just a scale).

In[∘]:= functionNz[z_, tscale_, jmax_, Nave_] := $\sum_{j=1}^{jmax} \frac{z^j}{\left(1 - Exp\left[\frac{-j}{tscale}\right]\right)^3}$ - Nave

In[∘]:=

```
Plot[{functionNz[z, 0.4, 100, 100],
  functionNz[z, 0.4, 500, 100], functionNz[z, 0.4, 1000, 100]}, {z, -1.1, 1}]
```

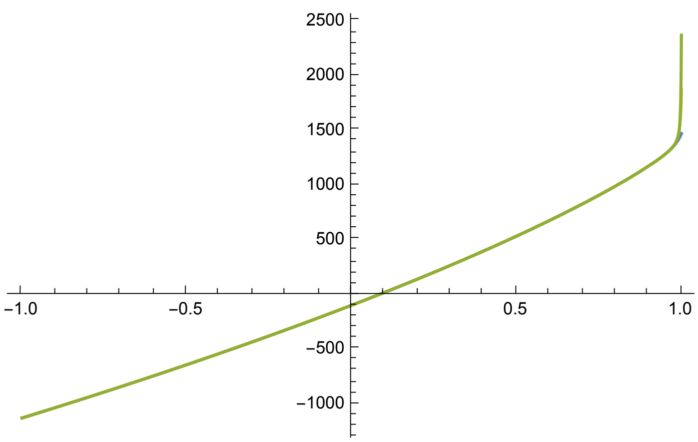
Out[∘]=



In[∘]:=

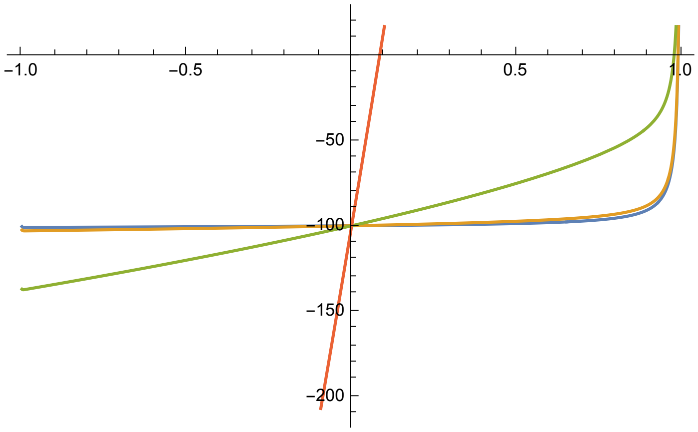
```
Plot[{functionNz[z, 10., 100, 100],
  functionNz[z, 10., 500, 100], functionNz[z, 10., 1000, 100]}, {z, -1, 1}]
```

Out[∘]=



In[∘]:=
```
Plot[{functionNz[z, .5, 500, 100], functionNz[z, 1., 500, 100],
  functionNz[z, 3., 500, 100], functionNz[z, 10., 500, 100]}, {z, -1, 1}]
```

Out[∘]=



In[∘]:=

```
FindRoot[functionNz[z, .5, 2000, 100] == 0, {z, .98, 1}]
```

General: Exp[−710.] is too small to represent as a normalized machine number; precision may be lost.

General: Exp[−712.] is too small to represent as a normalized machine number; precision may be lost.

General: Exp[−714.] 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[∘]= {z → 0.990039}

In[∘]:=

```
FindRoot[functionNz[z, 10., 2000, 100] == 0, {z, 0, 1}]
```

Out[∘]= {z → 0.0850988}

In[∘]:=

$$\text{Tc0[N\_]} := \left(\frac{\text{N}}{\text{Zeta[3]}}\right)^{1/3}$$

In[∘]:=

```
ListFugacity = {};
ListN0overN = {};
ListChemPot = {};
Do[fugacity = z /. FindRoot[functionNz[z, Tcurrent, 2000, 100] == 0, {z, -0.2, 1}];
 AppendTo[ListN0overN, {Tcurrent / Tc0[100], fugacity/(1 - fugacity) / 100}];
 AppendTo[ListFugacity, {Tcurrent / Tc0[100], fugacity}];
 AppendTo[ListChemPot, {Tcurrent / Tc0[100], Tcurrent Log[fugacity]}],
 {Tcurrent, 0.5, 20, 0.1}]
```

··· General: Exp[−710.] is too small to represent as a normalized machine number; precision may be lost.

··· General: Exp[−712.] is too small to represent as a normalized machine number; precision may be lost.

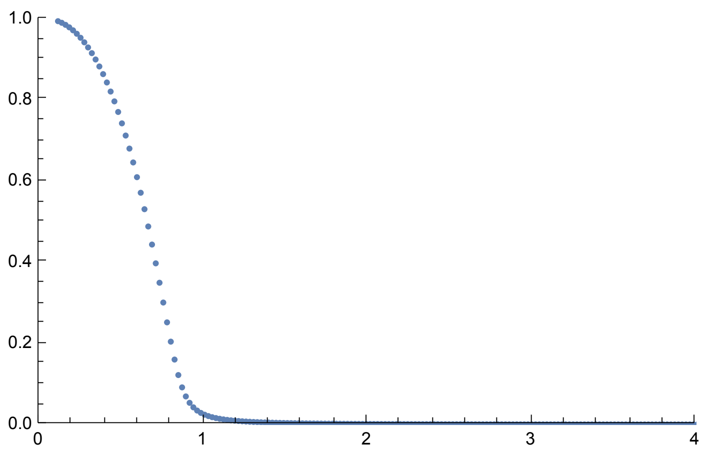
··· General: Exp[−714.] is too small to represent as a normalized machine number; precision may be lost.

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

In[∘]:=

```
ListPlot[ListN0overN, PlotRange → {{0, 4}, {0, 1}}]
```

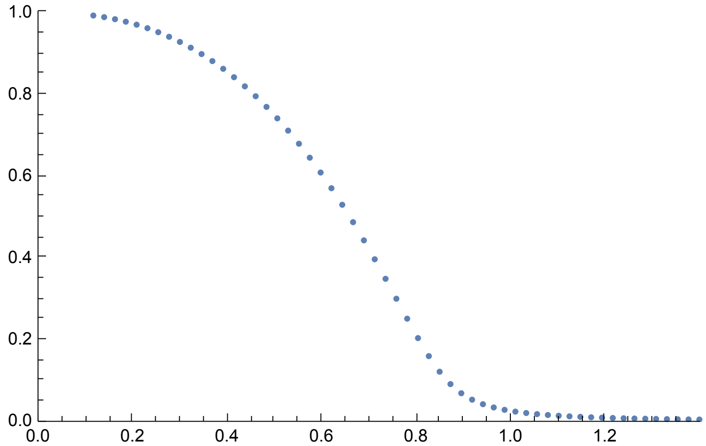
Out[∘]=



In[∘]:=

```
ListPlot[ListN0overN, PlotRange → {{0, 1.4}, {0, 1}}] (*Problem 3: Figure 1(a)*)
```

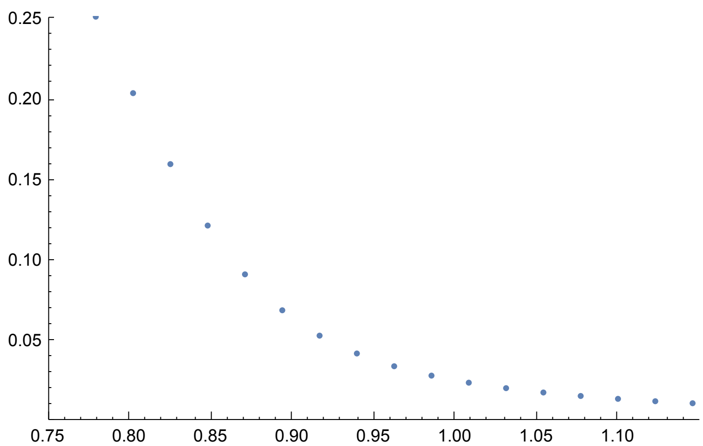
Out[∘]=



In[∘]:=

```
ListPlot[ListN0overN, PlotRange → {{0.75, 1.15}, {0, 0.25}}]
(*Problem 3: Figure 1(b)*)
```

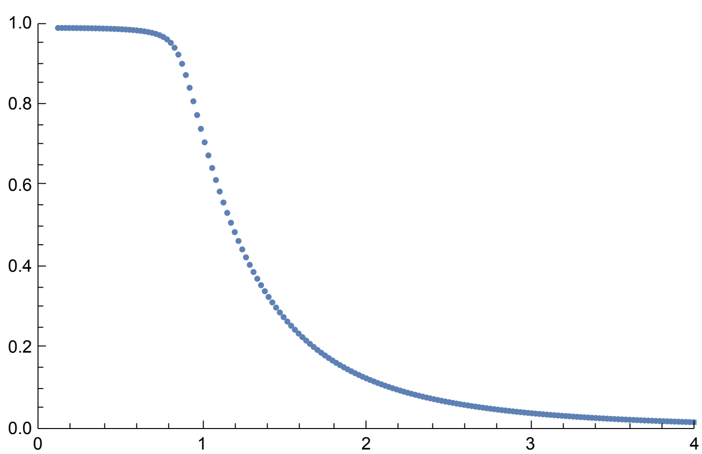
Out[∘]=



In[∘]:=

```
ListPlot[ListFugacity, PlotRange → {{0, 4}, {0, 1}}](*Problem 4*)
```

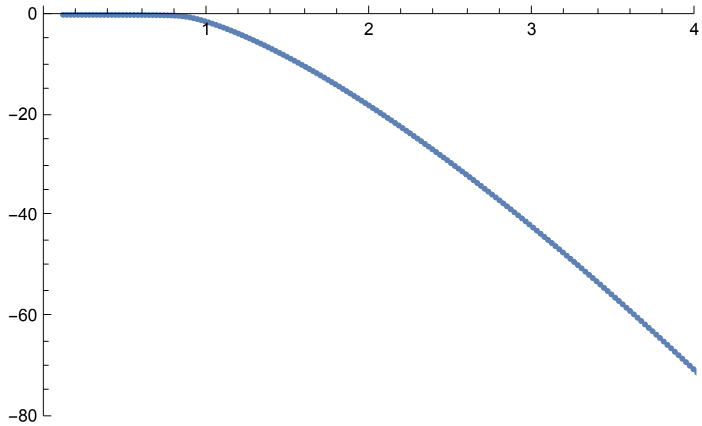
Out[∘]=



In[∘]:=

```
ListPlot[ListChemPot, PlotRange → {{0, 4}, {-80, 0}}](*Problem 4*)
```

Out[∘]=



In[∘]:=

```
ListPlot[ListChemPot, PlotRange → {{0, 1}, {-1, 0}}]
```

Out[∘]=