PHYS 5130 Problem Set 6 Solution

1.

Solution: In the question, the function to be minimized is

$$f(x, y, z) = x^2 + y^2 + z^2, \tag{1}$$

subject to the constraint that

$$g(x, y, z) = x^2 + y^2 - 2xz = 4. \tag{2}$$

Therefore, by the method of Lagrange multiplier, one could obtain the follow set of equations

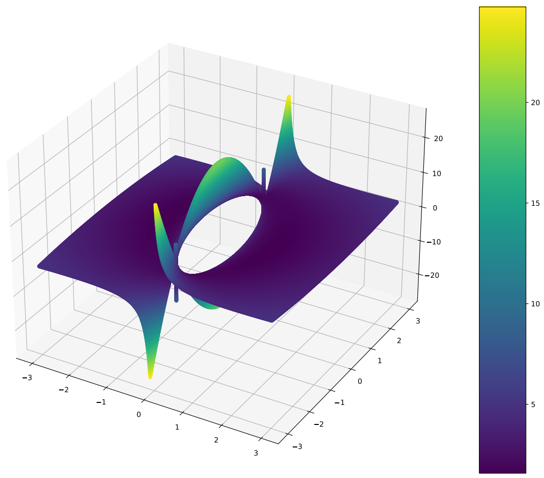
$$\begin{cases} 2x = \lambda(2x - 2z) \\ 2y = \lambda(2y) \\ 2z = \lambda(-2x) \\ x^2 + y^2 - 2xz = 4 \end{cases} . \tag{3}$$

From $2y = \lambda 2y$, and assuming $y \neq 0$, one obtains $\lambda = 1$. Substituting $\lambda = 1$ back into the equations, one could see that $x = z = 0$ and $y = \pm 2$, then $f(0, \pm 2, 0) = 4$, so the distance $d = 2$.

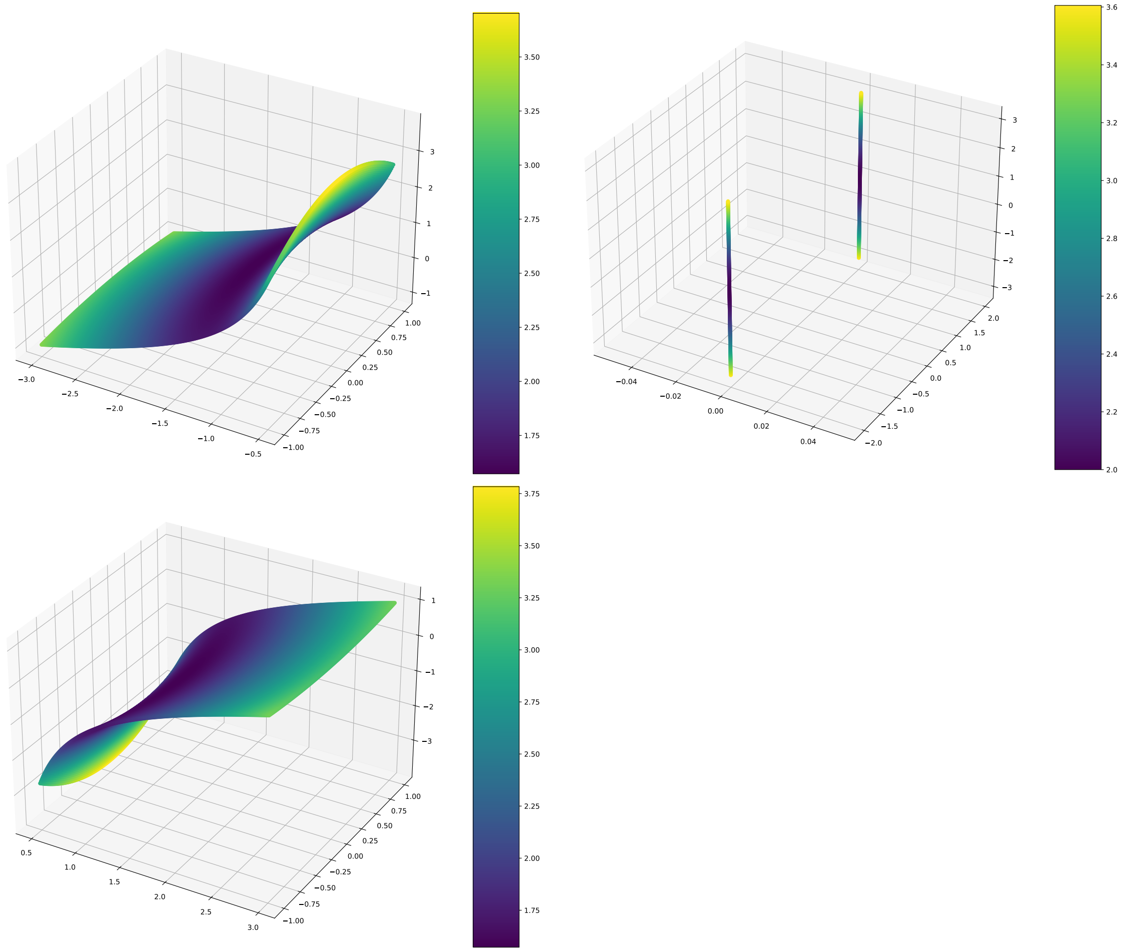
For $y = 0$, $z = -\lambda x$. Substituting it back into $2x = \lambda(2x - xz)$ and $x^2 + y^2 - 2xz = 4$, one obtains $x(1 - \lambda - \lambda^2) = 0$, and $x^2(1 + 2\lambda) = 4$, so $x \neq 0$. Therefore, $1 - \lambda - \lambda^2 = 0$. Solving the quadratic equation and taking the positive root, one obtains $\lambda = \frac{\sqrt{5}}{2} - \frac{1}{2}$, and so $x = \pm \frac{2}{5^{\frac{1}{4}}}$ and $z = \pm(5^{-\frac{1}{4}} - 5^{\frac{1}{4}})$, then $f = 2\sqrt{5} - 2$, and $d = 1.5723$.

So the minimum distance is $d = 1.5723$.

The figures below depict the surface $g(x, y, z) = 4$, with the colour indicating the distance from origin (d) of each position. One could see that the surface is split into three regions, $x < 0$, $x = 0$, $x > 0$.



Each part of the discontinuous surface contains one local minimum, which corresponds to the one of the positions and one of the distances obtained above.



2.

Solution: In this question, the quantity to be maximized is the number of microstates

$$g(\mathcal{N}_1, \mathcal{N}_2, \dots) = \ln\left(\frac{N!}{\mathcal{N}_1 \mathcal{N}_2 \dots}\right), \tag{4}$$

subject to the constraints

$$\begin{cases} f_1(\mathcal{N}_1, \mathcal{N}_2, \dots) = \sum_i \mathcal{N}_i = N \\ f_2(\mathcal{N}_1, \mathcal{N}_2, \dots) = \sum_i E_i \mathcal{N}_i = \mathcal{E} \end{cases}. \tag{5}$$

(a) Making using of Stirling approximation, $\ln N! = N \ln N - N$, $g \approx N \ln N - N - \sum_i (\ln \mathcal{N}_i - \mathcal{N}_i)$. By the method of Lagrange multiplier, one obtains the following system of equations

$$\begin{cases} -\ln \mathcal{N}_1 = \alpha + \beta E_1 \\ -\ln \mathcal{N}_2 = \alpha + \beta E_2 \\ \vdots \\ \sum_i \mathcal{N}_i = N \\ \sum_i E_i \mathcal{N}_i = \mathcal{E} \end{cases}. \tag{6}$$

Therefore,

$$\mathcal{N}_i = e^{-\alpha - \beta E_i}. \tag{7}$$

(b) Substituting the expression for $\mathcal{N}_i$ obtained in part (a) into the constraint

$$\sum_i \mathcal{N}_i = N, \tag{8}$$

one obtains

$$\sum_i e^{-\alpha-\beta E_i} = N \tag{9}$$

$$e^{-\alpha}\sum_i e^{-\beta E_i} = N \tag{10}$$

$$e^{-\alpha} = \frac{N}{\sum_i e^{-\beta E_i}} \tag{11}$$

$$\alpha = \ln\left(\frac{\sum_i e^{-\beta E_i}}{N}\right) \tag{12}$$

(c) Using the obtained expression for $e^{-\alpha}$, one obtains

$$\mathcal{N}_i = e^{-\alpha-\beta E_i} \tag{13}$$

$$= \frac{N}{\sum_i e^{-\beta E_i}} e^{-\beta E_i} \tag{14}$$

$$= N\frac{e^{-\beta E_i}}{\sum_i e^{-\beta E_i}}. \tag{15}$$

One could then identify $\frac{\mathcal{N}_i}{N} = P_i = \frac{e^{-\beta E_i}}{\sum_i e^{-\beta E_i}}$ as derived previously in the lecture, and so one could then identify $\beta = \frac{1}{kT}$ and partition function $Z = \sum_i e^{-\beta E_i}$.

(d)

$$< E > = \frac{\mathcal{E}}{N} \tag{16}$$

$$= \frac{\sum_i E_i \mathcal{N}_i}{N} \tag{17}$$

$$= \frac{1}{Z}\sum_i E_i e^{-\frac{E_i}{kT}} \tag{18}$$

$$= \frac{1}{Z}(kT^2)\frac{\partial}{\partial T}\sum_i e^{-\frac{E_i}{kT}} \tag{19}$$

$$= \frac{kT^2}{Z}\frac{\partial Z}{\partial T} \tag{20}$$

$$= kT^2\frac{\partial \ln Z}{\partial T} \tag{21}$$

3.

Solution:

$$S = \frac{S_{collection}}{N} \tag{22}$$

$$= \frac{k}{N}\ln W \tag{23}$$

$$= \frac{k}{N}(N\ln N - N - (\sum_i \mathcal{N}_i \ln \mathcal{N}_i - \mathcal{N}_i)) \tag{24}$$

As $N = \sum_i \mathcal{N}_i$, the above expression could further be written as

$$S = \frac{k}{N}(N \ln N - N - (\sum_i \mathcal{N}_i \ln \mathcal{N}_i - \mathcal{N}_i)) \tag{25}$$

$$= \frac{k}{N}\left((\sum_i \mathcal{N}_i \ln N) - \sum_i \mathcal{N}_i \ln \mathcal{N}_i\right) \tag{26}$$

$$= \frac{k}{N}\sum_i \mathcal{N}_i \ln\left(\frac{N}{\mathcal{N}_i}\right) \tag{27}$$

$$= -k\sum_i \frac{\mathcal{N}_i}{N} \ln\left(\frac{N}{\mathcal{N}_i}\right) \tag{28}$$

$$= -k\sum_i P_i \ln P_i \tag{29}$$

From Thermodynamics, one knows that $F =< E > -TS$. Then,

$$F =< E > -TS \tag{30}$$

$$=< E > +kT\sum_i P_i \ln P_i \tag{31}$$

$$=< E > +kT\sum_i P_i \ln\left(\frac{e^{-\beta E_i}}{Z}\right) \tag{32}$$

$$=< E > -\sum_i E_i P_i - kT \ln Z \sum_i P_i \tag{33}$$

$$=< E > - < E > -kT \ln Z \tag{34}$$

$$= -kT \ln Z \tag{35}$$

4.

Solution: For a particle in a box of size L^d, one could analytically solve for the eigenfunctions and eigenenergies, given by

$$\epsilon_{n_1,n_2,\dots,n_d} = \frac{\pi^2\hbar^2}{2mL}\sum_i^d n_i^2. \tag{36}$$

So that in terms of k, where $k_i = \frac{\pi n_i}{L}$,

$$\epsilon_{k_1,k_2,\dots,k_d} = \frac{\hbar^2}{2m}\sum_i^d k_i^2. \tag{37}$$

Then, one could obtain $g^<(k)$, which is the number of states with $\sqrt{\sum_i^d k_i^2} \leq k$.

$$g^<(k) = g_s \frac{V_d(k)}{2^d\left(\frac{\pi}{L}\right)^d} \tag{38}$$

$$= g_s \frac{\pi^{\frac{d}{2}} k^d L^d}{2^d \pi^d \Gamma(\frac{d}{2}+1)} \tag{39}$$

$$= g_s \frac{k^d L^d}{2^d \pi^{\frac{d}{2}} \Gamma(\frac{d}{2}+1)} \tag{40}$$

$$g^<(\epsilon) = g_s \frac{L^d}{2^d \pi^{\frac{d}{2}} \Gamma(\frac{d}{2}+1)}\left(\frac{2m\epsilon}{\hbar^2}\right)^{\frac{d}{2}} \tag{41}$$

$$= g_s \left(\frac{L^2 m}{2\pi\hbar^2}\right)^{\frac{d}{2}} \frac{\epsilon^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}. \tag{42}$$

Then, $g(\epsilon)$ could also be obtained,

$$g(\epsilon) = \frac{\partial g^<}{\partial \epsilon} \tag{43}$$

$$= g_s \left(\frac{L^2 m}{2\pi\hbar^2}\right)^{\frac{d}{2}} \frac{\frac{d}{2}\epsilon^{\frac{d}{2}-1}}{\Gamma\left(\frac{d}{2}+1\right)} \tag{44}$$

$$= g_s \left(\frac{L^2 m}{2\pi\hbar^2}\right)^{\frac{d}{2}} \frac{\epsilon^{\frac{d}{2}-1}}{\Gamma\left(\frac{d}{2}\right)}. \tag{45}$$

For $d = 3$,

$$g(\epsilon) = g_s \left(\frac{L^2 m}{2\pi\hbar^2}\right)^{\frac{3}{2}} \frac{\epsilon^{\frac{3}{2}-1}}{\Gamma\left(\frac{3}{2}\right)} \tag{46}$$

$$= g_s V \left(\frac{m}{2\pi\hbar^2}\right)^{\frac{3}{2}} \frac{\epsilon^{\frac{1}{2}}}{\frac{1}{2}\pi^{\frac{1}{2}}} \tag{47}$$

$$= g_s \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{\epsilon}, \tag{48}$$

of which is the same result as derived in the lecture.

Therefore, for n-dimensional ideal Fermi gas, one has the following equations

$$\begin{cases} N = \sum_i n_i = \sum_i g_i f_{FD}(\epsilon_i) = \int g(\epsilon) f_{FD}(\epsilon) d\epsilon \\ E = \sum_i \epsilon_i n_i = \sum_i \epsilon_i g_i f_{FD}(\epsilon_i) = \int \epsilon g(\epsilon) f_{FD}(\epsilon) d\epsilon \\ g(\epsilon) = g_s \left(\frac{L^2 m}{2\pi\hbar^2}\right)^{\frac{3}{2}} \frac{\epsilon^{\frac{3}{2}-1}}{\Gamma\left(\frac{3}{2}\right)} \end{cases} \tag{49}$$

5.

Solution: For ideal Bose gas, the number of microstates is given by

$$W = \prod_i \frac{(n_i + g_i - 1)!}{(g_i - 1)! n_i!} \approx \prod_i \frac{(n_i + g_i)!}{g_i! n_i!}, \tag{50}$$

where

$$\frac{n_i}{g_i} = f_{BE} = \left(e^{\frac{\epsilon - \mu}{kT}} - 1\right)^{-1}. \tag{51}$$

There, the entropy for ideal Bose gas is given by

$$S = k \ln W \tag{52}$$

$$= k \sum_i \ln\left(\frac{(n_i + g_i)!}{g_i! n_i!}\right) \tag{53}$$

$$= k \sum_i (n_i + g_i) \ln(n_i + g_i) - (n_i + g_i) - g_i \ln g_i + g_i - n_i \ln n_i + n_i \tag{54}$$

$$= k \sum_i n_i \ln(n_i + g_i) + g_i \ln(n_i + g_i) - g_i \ln g_i - n_i \ln n_i \tag{55}$$

$$= k \sum_i n_i \ln\left(1 + \frac{g_i}{n_i}\right) + g_i \ln\left(\frac{n_i}{g_i} + 1\right) \tag{56}$$

$$= k \sum_i n_i \left(\frac{\epsilon_i}{kT} - \frac{\mu}{kT}\right) + g_i \ln\left(\frac{n_i}{g_i} + 1\right) \tag{57}$$

$$= \frac{1}{T} \sum_i n_i \epsilon_i - \frac{1}{T} \sum_i n_i \mu + \sum_i g_i \ln\left(\frac{n_i}{g_i} + 1\right) \tag{58}$$

$$= \frac{< E >}{T} - \frac{\mu N}{T} + k \sum_i g_i \ln\left(\frac{n_i}{g_i} + 1\right). \tag{59}$$

From Thermodynamics,

$$S = \frac{< E >}{T} - \frac{\mu N}{T} + \frac{PV}{T}. \tag{60}$$

Therefore, one could identify

$$\frac{PV}{T} = k \sum_i g_i \ln\left(\frac{n_i}{g_i} + 1\right) \tag{61}$$

$$PV = kT \sum_i g_i \ln\left(\frac{n_i}{g_i} + 1\right) \tag{62}$$

$$= kT \sum_i g_i \ln\left(\frac{e^{\frac{\epsilon_i - \mu}{kT}}}{e^{\frac{\epsilon_i - \mu}{kT}} - 1}\right) \tag{63}$$

$$= -kT \sum_i g_i \ln\left(1 - e^{-\frac{\epsilon_i - \mu}{kT}}\right) \tag{64}$$