

25 Mar April

Logistics:

Homework returned

Final HW due 5, May

Final exam 14:30 Wed 1 June in Sports Centre

Recap:

Probability spaces  $\rightarrow$  statistical ensembles

Micro-canonical

Canonical

Grand-canonical

} Thermodynamic equilibrium

Partition Function & Free energy

Application: Classical ideal gases, thermodynamic cycles  
Quantum ideal gases of bosons & Fermions

# MATH327: Statistical Physics, Spring 2022

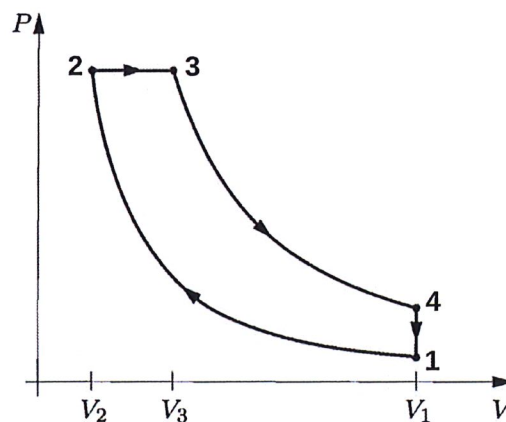
## Homework assignment 2

### Instructions

Complete all four questions below and submit your solutions by file upload on [Canvas](#).<sup>1</sup> Clear and neat presentations of your workings and the logic behind them will contribute to your mark. This assignment is **due by 23:59 on Thursday, 5 May**, and anonymous marking is turned on.

### Question 1: Thermodynamic cycle

Consider the Diesel cycle defined by the  $PV$  diagram shown below, in which the 'compression' stage  $1 \rightarrow 2$  and the 'power' stage  $3 \rightarrow 4$  are both adiabatic, while the pressure is constant during the 'injection/ignition' stage  $2 \rightarrow 3$ .



Calculate the efficiency of the Diesel cycle,  $\eta_D$ , in terms of the compression ratio  $r \equiv V_1/V_2 > 1$  and the cutoff ratio  $C \equiv V_3/V_2 > 1$ , where  $C < r$ .

[10 marks]

Fixing the compression ratio  $r$ , compare  $\eta_D$  to the efficiency of the Otto cycle. Is the Diesel cycle more efficient than the Otto cycle, less efficient, or the same? How does this depend on the cutoff ratio  $C$ ?

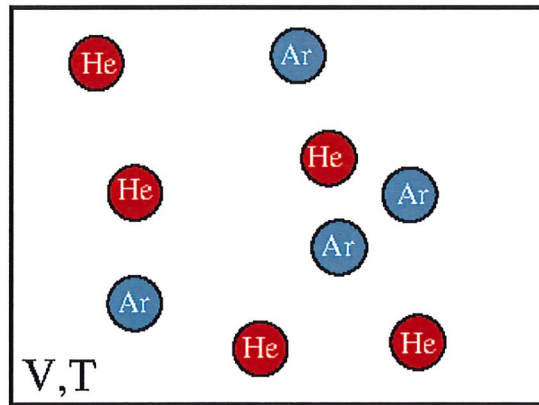
[4 marks]

<sup>1</sup>By submitting solutions to this assessment you affirm that you have read and understood the [Academic Integrity Policy](#) detailed in Appendix L of the Code of Practice on Assessment and have successfully passed the Academic Integrity Tutorial and Quiz. The marks achieved on this assessment remain provisional until they are ratified by the Board of Examiners in June 2022.

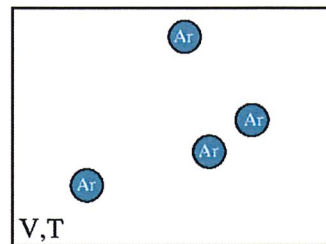
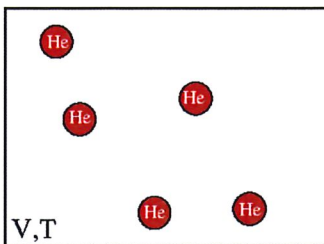
## Question 2: Mixed ideal gases

Consider a mixture of two ideal (non-interacting) gases in thermodynamic equilibrium in a container of volume  $V$  at temperature  $T$ , like that illustrated below. Let  $N_1$  and  $N_2$  be the fixed particle numbers of the two gases. Within each gas the particles are indistinguishable, but particles of one gas are distinguishable from particles of the other gas. In particular, they have different masses  $m_1$  and  $m_2$ , implying different thermal de Broglie wavelengths and single-particle canonical partition functions:

$$\lambda_i(T) = \sqrt{\frac{2\pi\hbar^2}{m_i T}} \quad Z_1^{(i)}(T) = \frac{V}{\lambda_i^3}$$



- (a) Calculate the canonical partition function  $Z$  and the Helmholtz free energy of the  $(N_1 + N_2)$ -particle mixture, approximating  $\log(N_i!) \approx N_i \log N_i - N_i$ . [4 marks]
- (b) Calculate the internal energy  $\langle E \rangle$  and the entropy  $S$  of the mixture. What is the condition of constant entropy? [4 marks]
- (c) Calculate the pressure  $P$  of the mixture, and relate it to the pressures  $P_1$  and  $P_2$  of each gas in isolation (as illustrated below). [4 marks]



### Question 3: Particle number fluctuations

Consider the fugacity expansion of the grand-canonical partition function (Eq. 82),

$$Z_g(T, \mu) = \sum_{N=0}^{\infty} \xi^N Z_N(T),$$

where the fugacity  $\xi = e^{\beta\mu} = e^{\mu/T}$  and  $Z_N(T)$  is the  $N$ -particle canonical partition function (which is independent of  $\xi$ ). Recall that  $\Phi(T, \mu) = -T \log Z_g(T, \mu)$  is the corresponding grand-canonical potential.

- (a) Derive a relation between the average particle number  $\langle N \rangle$  and the derivative  $\frac{\partial}{\partial \log \xi} \Phi = \xi \frac{\partial}{\partial \xi} \Phi$ .

[4 marks]

- (b) Derive a relation between  $\langle (N - \langle N \rangle)^2 \rangle$  and  $\left( \xi \frac{\partial}{\partial \xi} \right)^2 \Phi$ .

[4 marks]

- (c) Specializing to Maxwell–Boltzmann statistics, for which the fugacity expansion simplifies to  $Z_g^{\text{MB}}(T, \mu) = \exp[\xi Z_1(T)]$ , show

$$\frac{\sqrt{\langle (N - \langle N \rangle)^2 \rangle}}{\langle N \rangle} = \frac{1}{\sqrt{\langle N \rangle}}.$$

[4 marks]

As an aside, this final result means that the relative fluctuations in the particle number vanish in the **thermodynamic limit**  $\langle N \rangle \rightarrow \infty$ . That is, when  $\langle N \rangle$  is large it is approximately constant, which allows the grand-canonical system to be approximated by the corresponding canonical system with fixed  $N$ .

## Question 4: Magnetization

Consider a system of  $N$  (distinguishable) non-interacting 'spins' in a lattice at temperature  $T$ , where the value  $s_i$  of each spin can vary continuously in the range  $-1 \leq s_i \leq 1$ . In an external magnetic field of strength  $H > 0$ , the internal

energy of the system is  $E = -H \sum_{i=1}^N s_i$ .

- (a) Calculate the canonical partition function  $Z$  and the Helmholtz free energy of the system.

[4 marks]

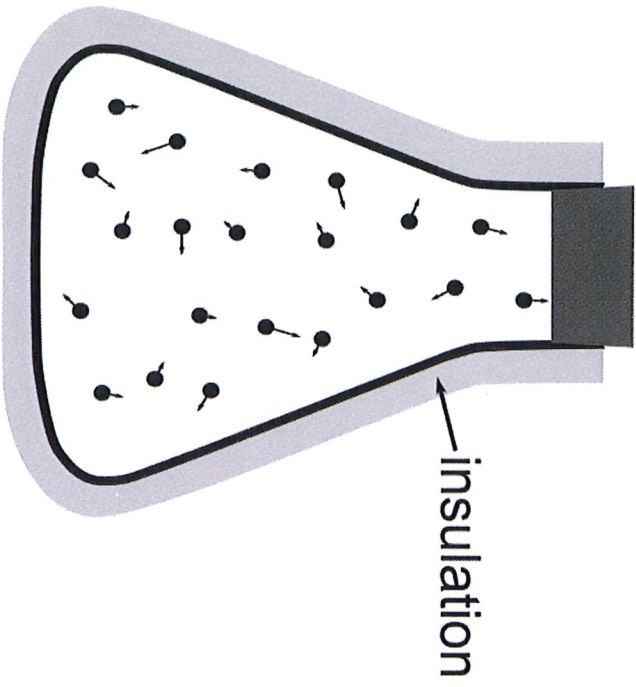
- (b) Calculate the magnetization  $\langle m \rangle$  of the system. For finite  $H > 0$ , what are its low- and high-temperature limits,  $\lim_{T \rightarrow 0} \langle m \rangle$  and  $\lim_{T \rightarrow \infty} \langle m \rangle$ ?

[4 marks]

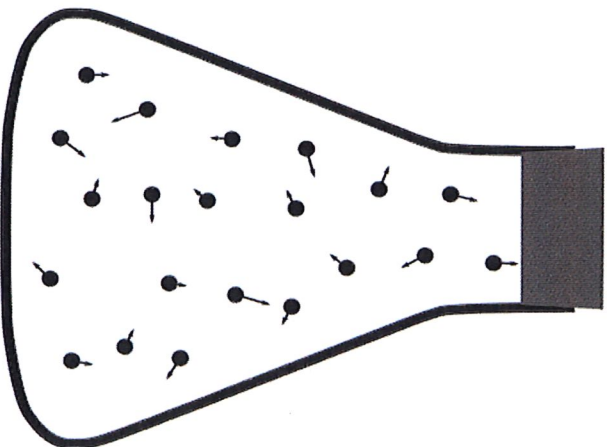
- (c) Calculate the leading  $T$ -dependent correction to each of the low- and high-temperature limits from the previous part.

[4 marks]

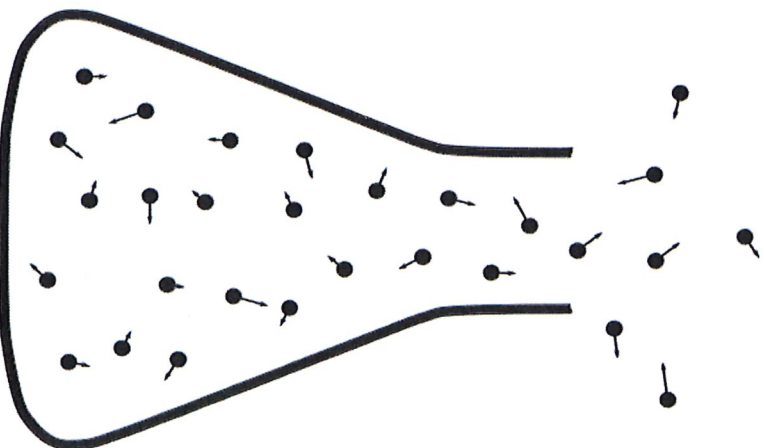




**Microcanonical**  
(const. N E)



**Canonical**  
(const. N T)



**Grand Canonical**  
(const.  $\mu$  T)

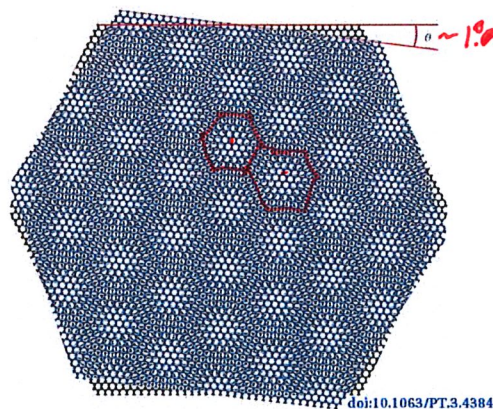
## Unit 9: Interacting systems

### 9.1 The Ising model

So far in this module we have considered ‘ideal’ systems composed of constituent degrees of freedom that do not interact with each other. While we have seen that this approximation of non-interacting particles can produce excellent mathematical models for real physical systems ranging from the low-temperature heat capacities of solids to solar radiation and the cosmic microwave background, there are crucial statistical physics phenomena that this approach fails to predict.

An important class of examples, which we investigate in this unit, are phase transitions. These occur when interactions allow extremely different large-scale behaviours to arise from the same set of degrees of freedom, depending on control parameters such as the temperature or pressure. Phase transitions occur in both everyday and extreme situations. Everyday examples include the liquid–gas transition of  $\text{H}_2\text{O}$  molecules from water to steam upon boiling a kettle, as well as the transition from liquid water to solid ice as the temperature decreases. In the extreme conditions following the big bang, the matter in the universe existed as a charged plasma of quarks and gluons. Once the universe was a few microseconds old, it cooled enough for this matter to transition into the protons and neutrons we are made out of today.

An intermediate example in between the everyday and the extreme involves two layers of graphene as illustrated in the figure below.<sup>12</sup> Graphene is an amazing material (recognized by the 2010 Nobel Prize in Physics) that consists of a single-atom-thick sheet of carbon atoms arranged in a hexagonal ‘honeycomb’ lattice. Under most conditions, graphene is an electrical insulator. However, if two graphene sheets are stacked and rotated with respect to each other by a small “magic angle”  $\theta \approx 1.1^\circ$ , the system transitions into a superconducting phase at low temperatures  $T \lesssim 1.7$  K. Superconductivity allows electrical current to flow with no resistance, meaning that no energy is lost to the production of waste heat. If we could discover or design materials that exhibit superconductivity at everyday temperatures  $T \sim 300$  K rather than low  $T \sim \mathcal{O}(1)$  K, it would revolutionize the energy efficiency of electronics and the power grid.



<sup>12</sup>Heather M. Hill, “[Twisted bilayer graphene enters a new phase](#)”, *Physics Today* **73**:18, 2020.

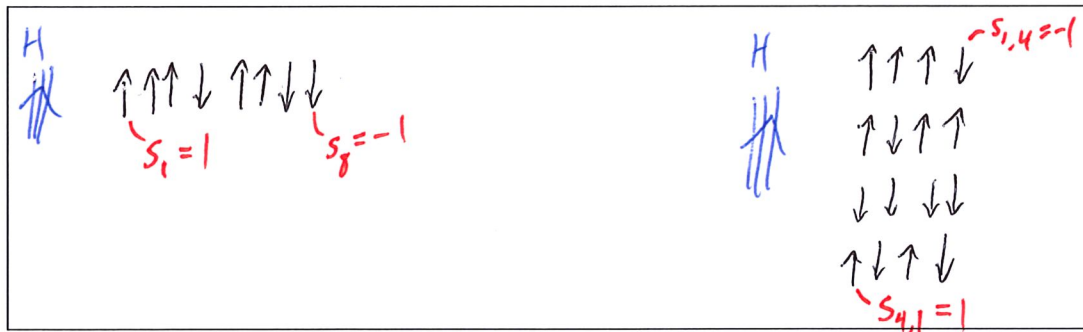


With this motivation for investigating phase transitions, let's step back to introduce interactions and explore their effects using simple spin systems of the sort we considered in units 2 and 3. In the non-interacting case we previously analyzed (Eq. 40), the internal energy of the system is

$$E_i = -H \sum_{n=1}^N s_n \quad (\text{non-interacting})$$

for micro-state  $\omega_i$  specified by the  $N$  spins  $\{s_n\}$  (and, as always for this module, in thermodynamic equilibrium). Here  $H > 0$  is the constant strength of an external magnetic field and the orientation of the  $n$ th spin,  $s_n$ , takes one of only two possible values:  $s_n = 1$  if the spin is aligned parallel to the field and  $s_n = -1$  if the spin is aligned anti-parallel to the field. The ground state of the system features all  $N$  spins aligned parallel to the magnetic field, with minimal energy  $E_0 = -NH$ .

In this unit we will only consider systems of distinguishable spins that we label by their fixed position in a  $d$ -dimensional simple cubic lattice. The  $d = 1$  case of a one-dimensional lattice is precisely the system of spins arranged in a line that we analyzed in Section 3.4.1. This and the case of  $d = 2$  are both easy to visualize and draw on a sheet of paper:



While we can only have physical lattices with  $d = 1, 2$  or  $3$  in nature, the mathematical construction works just as well for any integer  $d \geq 1$ .

We can see that the total internal energy of the non-interacting system can easily be written as a sum over energies  $\varepsilon_n$  for each individual spin,

$$\varepsilon_n = -H s_n \quad E_i = \sum_{n=1}^N \varepsilon_n \quad (\text{non-interacting}).$$

This is a generic feature of non-interacting systems, and an aspect of the factorization that enormously simplifies calculations — in this case by causing the  $N$ -particle partition function (Eq. 41) to take the form of a product of  $N$  identical terms,  $Z_N = [2 \cosh(\beta H)]^N = Z_1^N$ . However, it is possible to have non-factorizable systems in which the internal energy can be expressed as a sum of this sort. A stronger condition needs to be satisfied in order to guarantee factorization, and this conditions rigorously defines what it means for a system to be non-interacting.



Let  $\Delta E_j$  be the change in the system's internal energy caused by changing its  $j$ th degree of freedom. Then the system is defined to be **non-interacting** if and only if  $\Delta E_j$  for any  $j$  is independent of all other degrees of freedom  $k \neq j$ .

For our system of  $N$  distinguishable spins, the only possible change we can make to a degree of freedom is to negate it,  $s_j \rightarrow -s_j$ , which corresponds to flipping its alignment relative to the external magnetic field. It is easy to check that the change in the internal energy resulting from such a spin flip satisfies our definition of a non-interacting system:

$$E = -H \sum_n s_n = -H \left( s_j + \sum_{k \neq j} s_k \right) \rightarrow -H \left( -s_j + \sum_{k \neq j} s_k \right)$$

$$\Delta E_j = 2Hs_j \quad \text{independent of } s_k \text{ for } k \neq j$$

$$\rightarrow \text{non-interacting} \checkmark$$

Now let's make things more interesting by considering a different spin system that also includes a simple two-spin contribution to the internal energy:

$$E_i = - \sum_{(jk)} s_j s_k - H \sum_{n=1}^N s_n. \quad (111)$$

The first sum runs over all pairs of nearest-neighbour spins in the lattice, denoted  $(jk)$ . What is the change in energy  $\Delta E_j$  from Eq. 111 upon negating  $s_j \rightarrow -s_j$ ? Does this indicate an interacting or non-interacting system?

$$E = -s_j \sum_{k \in (jk)} s_k - \sum_{(mk) \neq j} s_m s_k - H \left( s_j + \sum_{k \neq j} s_k \right)$$

$$\rightarrow s_j \sum_{k \in (jk)} s_k - \sum_{(mk) \neq j} s_m s_k - H \left( -s_j + \sum_{k \neq j} s_k \right)$$

$$\left. \begin{array}{l} \\ \end{array} \right\} \Delta E_j = 2s_j \left( H + \sum_{k \in (jk)} s_k \right)$$

Depends on  $s_k$  with  $k \neq j$   
 $\rightarrow$  interacting

The pictures on the next page illustrate nearest-neighbour pairs for simple cubic lattices in  $d = 2$  and 3 dimensions, while also introducing some additional lattice terminology. Instead of drawing up- and down-pointing arrows, these pictures identify the spins with *sites* in the lattice represented as points (or larger filled circles). In simple cubic lattices, all sites are positioned in a regular grid, separated by a constant distance along each basis vector. We can also draw *links* as solid lines connecting these nearest-neighbour sites, with each link corresponding to a term in  $\sum_{(jk)}$ . The picture of a two-dimensional lattice on the left