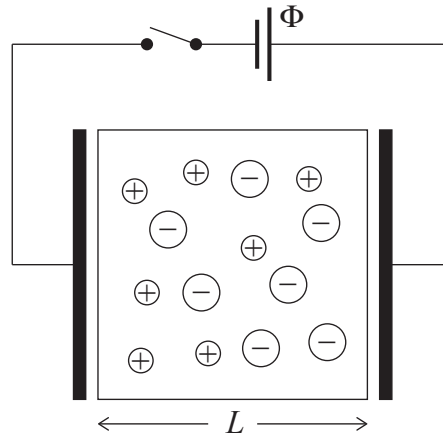


**Fig. 0.3** Illustration of system with charged particles in electric field. The system length is  $L$ .



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#### Exercise 0.8. Chemical potential in electrical field

We will address a system consisting of charged particles in a volume  $L^3$  as illustrated in Fig. 0.3.

The system as a whole is neutral (zero charge). When there is no external electrostatic field, the concentration of positive and negative charges is homogeneous and equal to  $n_0$ . We assume that the negative charges are immobile, but the positive are mobile, and that the concentration is so low that we can use ideal gas as an approximation. We apply an external field  $\Phi$  across the system through a pair of electrodes as illustrated in the figure, so that we get a directed electric field.

a) Set up an expression for the chemical potential of this system.

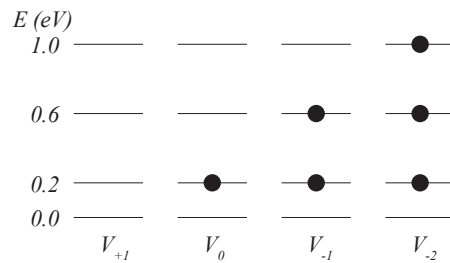
We assume that the system is electrically isolated, so there is no current after equilibrium is reached. Before the system reaches equilibrium, the mobile charges will move, changing the charge distribution,  $n(x)$ . According to Poisson's equation, this will also affect the field,  $\Phi(x)$ . The system reaches a stationary state in equilibrium, in which the functional forms of  $n(x)$  and  $\Phi(x)$  are unknown. The value of the potential at the electrodes are  $\Phi(L) = \Phi_L$  and  $\Phi(0) = \Phi_0 = 0$ .

b) What is the equilibrium condition?

c) Find the concentration of positive charges at the electrodes,  $n(0)$  and  $n(L)$ , expressed by  $\Phi_0$ ,  $\Phi_L$ ,  $n_0$  and  $T$ . You can assume that  $n(x)$  is an antisymmetric function about  $x = L/2$ .

d) How does the concentration qualitatively vary with  $x$ ? Make a sketch of  $n(x)$  to illustrate.

**Fig. 0.4** Illustration of how the occupation of various energy levels gives various charges for a vacancy.



e) (Difficult: May be used as basis for class discussion) Can you find a method to determine  $n(x)$  and  $\phi(x)$  numerically?

**Exercise 0.9.** Charged vacancies

We will study a system consisting of vacancies in crystalline Si. There are local energy states for the electrons associated with such a lattice defect. We assume that the vacancy can have four possible charge configurations with net charge +1, 0, -1, -2 when different levels are occupied by electrons. For simplicity, we will assume that one one-electron state is not affected by whether another state is occupied. We call the various charge-states  $V_1, V_0, V_{-1}, V_{-2}$ . The energy levels are sketched in Fig. 0.4. Assume that the energy for the vacancy is zero. Ignore the spin of the electron.

- Write down Gibbs sum for vacancies.
- Find the average charge state of the vacancy when the chemical potential for electrons,  $\mu = 0.2 \text{ eV}$ , at room temperature.
- What is the average charge state of the vacancy when the chemical potential is  $0.6 \text{ eV}$ .
- What is the average charge state of the vacancy when the chemical potential is  $1.1 \text{ eV}$  at low temperatures.

**Exercise 0.10.** Oxygen in the blood

*(This project is inspired by an exam in Fys114)*

In this project you will learn to apply Gibbs sum to address seemingly complex processes within a simple framework.

We will study a system of hemoglobin molecules in a liquid (such as blood). The liquid also contains dissolved  $\text{O}_2$ . A hemoglobin molecule may bind up to four oxygen molecules. We assume that each of the adsorption positions on the hemoglobin molecule are equivalent and indistinguishable. The binding energy for each  $\text{O}_2$  molecule is  $\varepsilon$  compared to the energy of an  $\text{O}_2$  molecule dissolved in the liquid. Each oxygen molecule can only have one possible orientation in each position.

- Write down an expression for Gibbs sum. Explain the symbols and the limits of the sums.

- b)** What is the probability,  $P(1)$ , that one, and only one,  $O_2$  molecule is adsorbed onto a hemoglobin molecule?
- c)** What is the probability,  $P(4)$ , that 4 (and only 4)  $O_2$  molecules are adsorbed on a hemoglobin molecule?
- d)** Plot  $P(1)$  and  $P(4)$  as a function of  $\lambda = \exp(\mu/kT)$ . Choose coordinates you find useful.
- e)** What are the limits for  $P(1)$  and  $P(4)$  when  $\lambda$  goes to zero and to its largest value?
- f)** Which probability is largest at large temperatures?

You can assume that the  $O_2$  in the liquid is in equilibrium with an ideal, diatomic gas of  $O_2$  outside the liquid.

- g)** How would the results change if you were on the top of Mount Everest?