Second Midterm Exam

P551

November 9, 2017

SHOW ALL WORK TO GET FULL CREDIT!

WARNING!!! Points will be taken if numerical calculations are nor provided and if calculations are left just indicated.

PART I: **DO IT IN CLASS** Turn your work in before leaving. Take the printed copy of the test home.

PART II: Take the test home and bring **ALL** the questions solved on Tuesday, November 14. Your grade for the test will be the **sum of the two** parts. A perfect score is worth 200 points as a result of 50 points to be earned in class and 150 points to be earned at home. If you are 100% sure about the work you did in class, you do not need to redo it at home. In that case the points obtained in class will be counted twice.

PART I

Problem 1: Consider a surface with sites that can absorb atoms. Each site can be empty, or have at most two atoms. The energy of the site is 0 if no atoms are absorbed, ϵ if there is only one atom, and 2ϵ if there are two atoms. The occupancy of the sites is not correlated. Assume that the system is in equilibrium with a reservoir at temperature T and chemical potential μ.

a) Write the grand-canonical partition function for one single site. (5 points)

b) Write the grand-canonical partition function for N sites. (5 points)

c) What is the mean number of atoms $\langle n \rangle$ that are absorbed per site as function of μ and T? (5 points)

d) What is $\langle n \rangle$ when $T = 0$? Does the result depend on whether $\epsilon > \mu$ and $\epsilon < \mu$? Why? (10 points)

e) What is $\langle n \rangle$ when $T \to \infty$? Does the result depend on whether $\epsilon > \mu$ and $\epsilon < \mu$? Why? (10 points)

f) If $\langle n \rangle = 0.5$ for $k_B T = 0.03$ eV and $\epsilon = 1$ eV. Find the value of the chemical potential μ. Hint: $k_B = 8.617 \times 10^{-5}$ eV/K. (10 points)

g) What is the average energy of the N site system in the conditions given in (f)? Give the result in eV. (5 points)

STOP HERE!!!!: Hand your work before leaving and take home the printed copy of the test. Bring **ALL** the questions answered on Tuesday, November 14.

PART II

Problem 1: Consider a surface with sites that can absorb atoms. Each site can be empty, or have at most two atoms. The energy of the site is 0 if no atoms are absorbed, ϵ if there is only one atom, and 2ϵ if there are two atoms. The occupancy of the sites is not correlated. Assume that the system is in equilibrium with a reservoir at temperature T and chemical potential μ.

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f) If $\langle n \rangle = 0.5$ for $k_B T = 0.03$ eV and $\epsilon = 1$ eV. Find the value of the chemical potential μ. Hint: $k_B = 8.617 \times 10^{-5}$ eV/K. (10 points)

g) What is the average energy of the N site system in the conditions given in (f)? Give the result in eV. (5 points)

h) Provide the probability of finding no absorbed atoms, one absorbed atom, and two absorbed atoms per site in the conditions given in (f). (5 points)

i) At what value of μ will the average value of absorbed atoms in the N site system be equal to N if $T = 0.03/k_B$ is kept fixed to the value in (f)? Give the result in eV. (5 points)

Problem 2: Consider N particles with quantum spin 1/2 defined in the basis $(|\uparrow\rangle_i, |\downarrow\rangle_i)$ for each particle labeled by the index i.

a) Consider the case in which $N = 3$. What will be the dimension of each of the single particle density matrices $\hat{\rho}_i$ and of the multiparticle density matrix ρ? (5 points)

b) Consider the case in which $N = 3$ and particles 1 and 2 are in the state $|\uparrow\rangle$ while particle 3 is in the state $|\downarrow\rangle$.

i) Write the single particle density matrix $\hat{\rho}_i$ for each of the three particles. (5 points)

ii) Provide an expression, in matrix form, for the multiparticle density matrix. (5 points)

iii) Calculate ρ^2. Do you expect that $\rho^2 = \rho$? Explain. (5 points)

iv) What is the entropy of this state? Why? (5 points)

c) Consider the case in which $N = 3$ and each particle is in the state $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$.

i) Write the single particle density matrix $\hat{\rho}_i$ for each of the three particles. (5 points)

ii) Provide an expression, in matrix form, for the multiparticle density matrix. (5 points)

iii) Calculate ρ^2. Do you expect that $\rho^2 = \rho$? Explain. (5 points)

iv) What is the entropy of this state? Why? (5 points)

d) Consider the case in which $N = 3$ and each particle has 50% probability of being in state $|\uparrow\rangle$ and 50% probability of being in state $|\downarrow\rangle$.

i) Write the single particle density matrix $\hat{\rho}_i$ for each of the three particles. (5 points)

ii) Provide an expression, in matrix form, for the multiparticle density matrix. (5 points)

iii) Calculate ρ^2. Do you expect that $\rho^2 = \rho$? Explain. (5 points)

iv) Use the density matrix to calculate the entropy of the state. (5 points)

e) Now write the partition function for the case of N particles in the canonical formalism assuming that the single particle Hamiltonian has eigenvalues $E_1 = -\epsilon$ and $E_2 = \epsilon$ ($\epsilon > 0$) and provide the probability of occupation of each single particle energy level:

i) At a generic temperature $T = (k\beta)^{-1}$. (5 points)

ii) At $T = 0K$. (5 points)

iii) At $T \to \infty$. (5 points)

iv) Can this system have a probability of occupancy of 40% for the lowest energy level and 60% for the highest one? What would be the temperature in that situation? Explain.(10 points)