Department of Physics
The Ohio State University

Prof. R. Bundschuh

First Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important dates: Feb 10 10:30am-12:18pm midterm exam,
Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Jan 13

1. Review *10 points*

Let us start by reviewing some of the key concepts from the first statistical mechanics course.

a) What are the three laws of thermodynamics?

b) What is special about the entropy in thermodynamic equilibrium compared to all other possible states of a system?

c) What is a thermodynamic phase transition and what is the difference between a first-order and a continuous phase transition?

d) What is the relation between the entropy of a macroscopic state and the number of microscopic states which correspond to the macroscopic state?

e) What is the probability distribution of the microcanonical ensemble? What physical situation does it correspond to?

2. Harmonic oscillators *10 points*

Let us consider an Einstein solid and look at it from a classical point of view. The Einstein solid picture assumes that atom i of a solid sits at lattice position $\vec{r}_{0,i}$ and can oscillate harmonically around this position. It is described by the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} + \frac{1}{2} m\omega^2 \sum_{i=1}^{N} (\vec{r}_i - \vec{r}_{0,i})^2.$$

a) What shape does the phase space volume with energy less than E, i.e., the volume $H(\vec{x}^N) \le E$ have?

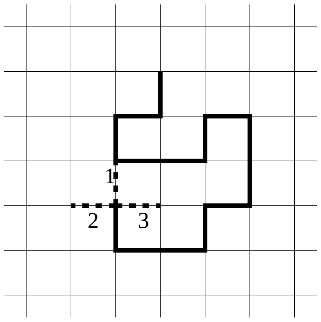
b) Calculate the entropy S of the Einstein solid at a given energy E using classical theory. When you evaluate the constant C_N take into account, that the oscillators have different origins and thus the atoms are distinguishable!

c) In what limit does your result coincide with the quantum mechanical result derived in last quarter's lecture? (You can find last quarter's lecture on the Einstein solid at `http://cannoli.mps.ohio-state.edu/phy846/phy846-14.pdf`)

d) What would the entropy be, if we had a gas of N particles within *the same* harmonic oscillator, i.e., if $\vec{r}_{0,i} = 0$ for all i. Is this entropy an extensive quantity? (Hint: You have to use a different constant C_N.)

3. A polymer on the lattice - microcanonical *10 points*

To appreciate the differences between the microcanonical and the canonical ensemble we want to solve one more problem in the microcanonical ensemble. A simple model for a polymer in two dimensions is that of a path on a square lattice. At every lattice point the polymer can either go straight (option 1 in the figure) or choose between the two directions in a right angle with respect to its current direction (options 2 and 3 in the figure.) Each time it bends in a right angle, it pays a bending energy ϵ. Thus, for a given "shape" of the polymer the total bending energy of the polymer is ϵ times the number of right angle turns. We assume that the starting segment of the polymer is fixed somewhere on the lattice and that the polymer consists of $N+1$ segments. Each possible shape of the polymer is a state of this statistical mechanics system.



a) How many polymer shapes have a total bending energy E where we assume $E = m\epsilon$ with some integer $0 \leq m \leq N$? (Hint: First count how many ways there are to position the m right angles on the polymer of length $N+1$ segments and then take into account that there are 2 possible choices for each right angle, namely left and right.)

b) What is the entropy $S(E, N)$ of this system? Approximate all factorials with the help of Stirling's formula.

c) Calculate the temperature of this system as a function of the total bending energy E and the length N of the polymer.

d) Calculate the energy E of the polymer as a function of the temperature T and of the length N of the polymer.

e) Calculate the heat capacity at constant length C_N as a function of the temperature T and the length N of the polymer.

Department of Physics
The Ohio State University
Prof. R. Bundschuh

Second Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important dates: Feb 10 10:30am-12:18pm midterm exam,
Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Jan 20

4. Two-state system

8 points

A (very small) discrete system has only two states 1 and 2 with energies $E_1 = -\varepsilon_0$ and $E_2 = \varepsilon_0$, respectively. This could, e.g., be a spin 1/2 particle in an external magnetic field. Since this system contains only one particle, the different thermodynamic ensembles do *not* provide equivalent descriptions of the physics. We want to explore this difference for this simplest possible system.

a) If the system is isolated from the environment which are the possible values for the internal energy of the system?

b) In the following we assume that the system is not isolated any more but instead interacting with a heat bath of temperature T. What are the probabilities p_i to find the system in each of the two states in this case.

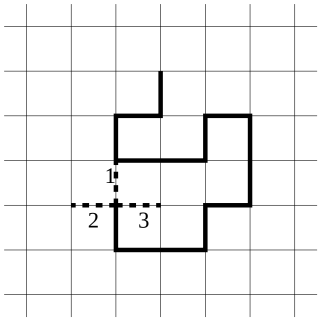
c) Calculate the internal energy as a function of the temperature of the heat bath.

d) Which are the possible values for the internal energy of the system when coupled to the heat bath? Consider the limiting values of the expression you calculated in c).

5. A polymer on the lattice - canonical

10 points

In order to compare the different ensembles we want to study the two dimensional polymer from problem 3 in the canconical ensemble. Again, we model the polymer as a path on a square lattice. At every lattice point the polymer can either go straight (option 1 in the figure) or choose between the two directions in a right angle with respect to its current direction (options 2 and 3 in the figure.) Each time it bends in a right angle, it pays a bending energy ϵ. If it goes straight the energy contribution of the respective joint is zero. Thus, for a given "shape" of the polymer the total bending energy of the polymer is ϵ times the number of right angle turns. We assume that the starting segment of the polymer is fixed somewhere on the lattice and that the polymer consists of $N + 1$ segments. Each possible shape of the polymer is a state of this statistical mechanics system.



a) Calculate the partition function of this polymer as a function of temperature T and the number of joints N of the polymer.

b) Calculate the average internal energy U of this polymer as a function of temperature T and the number of joints N of the polymer.

c) Compare your result in b) with the result from problem 3d).

6. Barometric formula

10 points

We want to derive how the air pressure depends on the height above sea level. To make things simple we pretend that air consists of only one type of molecules of mass m. We consider a volume of gas over an area of size A at sea level. The z-coordinate of the molecules has to be positive (i.e., above sea level) but is otherwise unconstrained. There are N molecules in this volume. The energy of the gas is given by

$$H(\vec{x}^N) = \begin{cases} \sum_{i=1}^{N} \left[\frac{\vec{p}_i^2}{2m} + mgz_i \right] & \text{all } z_i \geq 0 \text{ and } (x_i, y_i) \text{ within area } A \\ +\infty & \text{otherwise} \end{cases},$$

where $\vec{r_i} = (x_i, y_i, z_i)$ are the coordinates of molecule i.

a) Calculate the partition function $Z(T)$ of the gas.

b) The probability density $\rho(\vec{r})$ to find *some* particle of the gas at position $\vec{r}$ is given by

$$\rho(\vec{r}) = \int d\vec{x}^N \rho(\vec{x}^N) \delta(\vec{r}_1 - \vec{r})$$

where $\vec{r}_1$ is the position of particle 1. Calculate this probability density by performing the integral.

c) Use the law of large numbers and the ideal gas law $PV = Nk_BT$ applied to the volume $V = A\Delta z$ for a small height slice of thickness Δz in order to relate the probability density $\rho(\vec{r})$ to the pressure $P(z)$ at height z.

Department of Physics
The Ohio State University
Prof. R. Bundschuh

Third Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important dates: Feb 10 10:30am-12:18pm midterm exam,
Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Jan 27

7. Ultra-relativistic gas *12 points*

If the particles of a gas have velocities close to the speed of light c, their energy has to be calculated relativistically. In the limit of massless particles (e.g., photons) which travel at the speed of light, this relation between the momentum $\vec{p}_i$ of particle i and its energy E_i becomes $E_i = c|\vec{p}_i|$. Thus, the energy of a gas of N of these particles in a box of volume V is

$$H(\vec{x}^N) = \begin{cases} c\sum\limits_{i=1}^{N} |\vec{p}_i| & \text{all } \vec{r}_i \text{ inside volume } V \\ +\infty & \text{otherwise} \end{cases} .$$

a) Calculate the partition function of such an ultra-relativistic gas. (Hint: $\int\limits_0^\infty x^2 \exp(-x) dx = \Gamma(3) = 2$.)

b) Calculate the free energy of the ultra-relativistic gas as a function of its natural variables temperature T, volume V, and number of particles N. Use Stirling's formula to express your result in an explicitely extensive form.

c) Derive the equation of state (i.e., the relation between pressure P, volume V, temperature T, and number of particles N) of the ultra-relativistic gas.

d) Express the internal energy U of the ultra-relativistic gas in terms of the temperature T and the number of particles N.

8. Rubber elasticity *12 points*

As a simple model of an elastic string like, e.g., a rubber band, we consider a linear chain of N building blocks. Each building block can be in two different states a or b. In these states the building blocks have length l_a, and l_b and energies ε_a and ε_b, respectively. The total length of the chain is $L = N_a l_a + N_b l_b$ and the total energy of the string by itself is $E_0 = N_a \varepsilon_a + N_b \varepsilon_b$ where $N_a = N - N_b$ is the number of building blocks in state a. The string is streched by an external force f which turns the total energy of a state into $E = E_0 - Lf$.

a) Calculate the partition function of this string as a function of temperature T, the number of building blocks N, and the external force f. Introduce variables $n_i \in \{a, b\}$ that describe in which state building block i is and write the partition function as a sum over these variables n_i.

b) Calculate the average internal energy U of this string as a function of temperature T, the number of building blocks N, and the external force f.

c) Calculate the expected length $\langle L \rangle$ of this string as a function of temperature T, the number of building blocks N, and the external force f. (Hint: The expected length is a similar quantity as the expected energy. Find an expression for the expected length through a derivative similar to the derivative which we use to calculate the average internal energy.) What is the expected length at zero force in the case $\varepsilon_a = \varepsilon_b$? Why?

9. Relative momentum

10 points

We calculated in the lecture the distribution of velocities of the molecules of an ideal gas. In addition we would like to know how the *relative momentum* of two particles of the ideal gas is distributed. We concentrate on the absolut value $p_r \equiv |\vec{p}_i - \vec{p}_j|$ of this relative momentum. Calculate the probability density $P_{P_r}(p)$ of p in an ideal gas. (Hint: at some point you are left with an integral over the momenta of two different particles. It is is useful to transform this integral to a "center of mass" and a "relative" momentum in the same way as this is done in classical mechanics for coordinates, i.e., $\vec{P} = (\vec{p}_i + \vec{p}_j)/2$ and $\vec{p} = \vec{p}_i - \vec{p}_j$.)

Department of Physics
The Ohio State University

Prof. R. Bundschuh

Fourth Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important dates: Feb 10 10:30am-12:18pm midterm exam,
Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Feb 3

10. A two-dimensional solid

10 points

Consider a two-dimensional lattice in the x-y-plane with sides of length L_x and L_y which contains N atoms (N very large) coupled by nearest-neighbor harmonic forces.

a) Compute the Debeye frequency for this lattice. Note, that although the atoms are in a two-dimensional lattice they can still oscillate in three space directions. However, in a planar solid, there are three sound velocities: one transversal within the plane of the solid, one transversal out of the plane of the solid, and one logitudinal.

b) Calculate the heat capacity of this solid. You may use the results from the lecture that are independent of the dimension of the solid without rederiving them.

c) What is the asymptotic behavior of the heat capacity for very large temperatures?

d) What is the asymptotic behavior of the heat capacity for very small temperatures? (Hint: $\int\limits_0^\infty dx x^3 \frac{\exp(x)}{(\exp(x)-1)^2} = 6\zeta(3)$.)

11. Rotational degrees of freedom

10 points

Hydrogen molecules can exists in two forms: ortho- and para-hydrogen.

a) The two electrons of H_2 in para-hydrogen form a singlet (antisymmetric) state. The orbital angular momentum can thus only take even values $E_p = \frac{\hbar^2}{2I}L(L+1)$, where $L = 0, 2, 4, \ldots$. Write down the rotational partition function of a single para-hydrogen. You will not be able to actually perform the sum which you get.

b) In ortho-hydrogen, the electrons are in triply degenerate states, hence $E_o = \frac{\hbar^2}{2I}L(L+1)$, where $L = 1, 3, 5, \ldots$. Write down the rotational partition function of a single ortho-hydrogen. Do not forget the factor of three representing the degeneracy of the electronic states.

c) For an equilibrium gas of N hydrogen molecules (which contains both para- and ortho-hydrogen), calculate the total partition function coming from the rotational degrees of freedom. (Hint: Sum over contributions from mixtures of N_p para- and $N_o = N - N_p$ ortho-hydrogen particles.)

d) Write down the expression for the rotational contribution to the internal energy $\langle E_{rot} \rangle$, and discuss its low and high temperature limits. (Hint: at high temperatures you can replace the sum by an integral but you should say why.)

12. DNA denaturation *12 points*

DNA is a long molecule consisting of N units called "bases". The natural state of a DNA molecule in a cell is a configuration in which two of these DNA molecules are bound together base by base, i.e., base 1 of the first molecule is bound to base 1 of the second molecule, base 2 of the first molecule is bound to base 2 of the second molecule and so on. In this state the DNA takes on its well-known double helical structure. Chemical differences between the bases prevent the bases at different positions to bind to each other. If temperature rises these bindings can break up. We want to describe this process. To this end, we assign a variable s_i, $i \in \{1, \ldots, N\}$ to each of the N bases of one of the molecules. s_i can take the values 0 and 1. $s_i = 1$ means that the base is bound to its partner base in the other molecule; $s_i = 0$ means that the base is unbound. There are two energetic contributions in this system: A bound pair of bases gains a binding energy ε_0. In addition, there is an energy gain of ε_s whenever two neighboring bases are bound. The latter results from a favorable interaction between neighboring bases of the same molecule which can occur only if both bases are bound to the corresponding bases in the other molecule. The total binding energy of a configuration $(s_1, \ldots, s_N)$ is

$$H(s_1, \ldots, s_N) = -\varepsilon_0 \sum_{i=1}^{N} s_i - \varepsilon_s \sum_{i=1}^{N} s_i s_{i+1}.$$

We assume that the DNA molecule is closed to a ring, i.e., that $s_{N+1} = s_1$ (this is indeed the case for bacterial genomes.)

a) Calculate the partition function of this system in the limit of very long molecules.

b) Calculate the fraction of bound bases. Since the number of bound bases in a given configuration is given by $\sum_{i=1}^{N} s_i$, the fraction of bound bases is $\langle \sum_{i=1}^{N} s_i \rangle / N = \langle s_1 \rangle$ where the equality is due to the translational invariance. Since in reality $\varepsilon_0 \ll \varepsilon_s$, we can set $\varepsilon_0 = 0$ in the result.

c) Calculate the heat capacity of such a pair of DNA molecules at $\varepsilon_0 = 0$.

d) Plot the fraction of bound bases and the heat capacity as functions of dimensionless temperature $k_B T / \varepsilon_s$ at $\varepsilon_0 = 0$.

Department of Physics
The Ohio State University

Prof. R. Bundschuh

Fifth Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important dates: Feb 10 10:30am-12:18pm midterm exam,
Mar 16 9:30am-11:18am final exam

Due date: Thursday, Feb 12

13. Spin correlations *8 points*

Consider a one-dimensional lattice with N lattice sites and assume that the ith lattice site has spin $s_i = \pm 1$. The Hamiltonian describing this lattice is $H = -\varepsilon \sum_{i=1}^{N} s_i s_{i+1}$. Assume periodic boundary conditions, so $s_{N+1} \equiv s_1$. Compute the correlation function $\langle s_1 s_2 \rangle$. How does it behave at very high temperature and at very low temperature?

14. Spin 1 magnet *12 points*

Consider a lattice of N spins s_i which can take values $s_i \in \{-1, 0, 1\}$. In the absence of an external magnetic field the energy of this system is given by

$$H = -\varepsilon \sum_{\{i,j\}} s_i s_j.$$

Apply the mean field approximation to this system. Denote the number of nearest neighbors of a spin by ν.

a) At which temperature T_c does the system have a phase transition?

b) How does the magnetization behave at $T > T_c$, at $T \to 0$, and at $T \approx T_c$ but $T < T_c$

c) Calculate the heat capacity in the three temperature regimes given in b).

15. Ideal gas — grand canonical ensemble *12 points*

As the simplest example for the grand canonical ensemble, we want to study the ideal gas again. The energy of an ideal gas is given by

$$H(N, \vec{x}^N) = \sum_{j=1}^{N} \frac{\vec{p}_j^2}{2m}.$$

a) Calculate the grand canonical partition function of the ideal gas.

b) Calculate the grand canonical potential of the ideal gas as a function of temperature T, volume V, and chemical potential μ'.

c) Verify the ideal gas law $PV = Nk_BT$ by taking appropriate derivatives of the grand canonical potential. (Hint: P and N are given by one derivative each.)

d) Calculate $\langle N^2 \rangle - \langle N \rangle^2$ by taking a suitable derivative of the grand canonical potential. Express the relative fluctuation $\sqrt{\langle N^2 \rangle - \langle N \rangle^2}/N$ of the number of particles as a function of temperature T, volume V, and the number of particles N. How large is this relative fluctuations for 1 mole $(6 \cdot 10^{23})$ of particles?

Department of Physics
The Ohio State University

Prof. R. Bundschuh

Sixth Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important date: Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Feb 17

16. Adsorption to a surface

10 points

Consider a solid surface to be a two-dimensional lattice with M sites. Each site can be either empty or occupied with a single adsorbed atom. An adsorbed atom has a binding energy $-\varepsilon$ and we neglect any interactions between the atoms.

a) Calculate the grand canonical partition function of the adsorbed atoms as a function of temperature T, lattice size M, and chemical potential μ'. Use variables $n_i \in \{0, 1\}$ for each $i = 1, \ldots, M$ to describe if site i is empty or occupied.

b) Calculate the grand canonical potential of the adsorbed atoms as a function of temperature T, lattice size M, and chemical potential μ'.

c) Calculate the average number of adsorbed atoms N as a function of temperature T, lattice size M, and chemical potential μ'.

d) The surface is exposed to an ideal gas of the atoms at some pressure P and the same temperature T as the surface. Calculate the fraction N/M of adsorbed atoms as a function of the pressure P of the ideal gas and the temperature T of the system. (Hint: in thermodynamic equilibrium the chemical potentials of the adsorbed atoms and the atoms in the ideal gas have to be equal.)

17. Density operator

10 points

a) In a two-dimensional Hilbert space an operator $\hat{\rho}$ is given by the matrix

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} 1 + a_1 & a_2 \\ a_3 & 1 - a_1 \end{pmatrix}.$$

Determine for which values of the three complex parameters a_1, a_2, and a_3 this operator is a density operator. For which values of the three parameters is it a pure state?

b) Prove that for a hermitian Hamiltonian $\hat{H}$ the operator $\hat{\rho} \equiv e^{-\beta \hat{H}} / \operatorname{tr} e^{-\beta \hat{H}}$ is a density operator.

Department of Physics
The Ohio State University

Prof. R. Bundschuh

Seventh Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important date: Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Feb 24

18. Spin 1 atom

12 points

An atom with spin 1 has a Hamiltonian $\hat{H} = A\hat{S}_z^2 + B(\hat{S}_x^2 - \hat{S}_y^2)$, where $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ are the x, y, and z component of the spin angular momentum operator. In the basis of eigenstates of the operator $\hat{S}_z$ these three operators have the matrix representations

$$\hat{S}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \hat{S}_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \text{and} \quad \hat{S}_y = \frac{\hbar}{i\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}.$$

At time $t = 0$ the atom is initially in an eigenstate of $\hat{S}_z$ with eigenvalue $+\hbar$.

a) Write the density matrix (in the basis of eigenstates of $\hat{S}_z$) at $t = 0$.

b) Compute the density matrix at time t in the basis of eigenstates of $\hat{S}_z$.

c) Compute the average z component of the spin at time t.

19. Extremality of density operators I

12 points

We want to look in more detail in which sense the density operators of the canonical and grand canonical ensemble maximize the entropy. To this end we want to prove the identity

$$\mathrm{Tr}\hat{\rho}_1(\ln\hat{\rho}_2 - \ln\hat{\rho}_1) \le 0 \tag{1}$$

for *any* pair of density operators ρ_1 and ρ_2. In the next problem we apply this identity to the canonical and the grand canonical density operators.

a) Use the Cauchy-Schwarz inequality applied to the scalar product $\langle\hat{A},\hat{B}\rangle \equiv \mathrm{Tr}AB^\dagger$ in order to prove $\mathrm{Tr}\hat{\rho}_1^{1/2}\hat{\rho}_2^{1/2} \le 1$. A fractional power of an operator is defined by $\hat{A}^x \equiv \exp(x\ln\hat{A})$ where exp and ln are defined by their power series.

b) Use induction on n in order to prove

$$\mathrm{Tr}(\hat{\rho}_1^{1-2^{-n}}\hat{\rho}_2^{2^{-n}}) \le 1$$

for any integer $n \ge 1$. (Hint: Rewrite $\hat{\rho}_1^{1-2^{-n}}\hat{\rho}_2^{2^{-n}} = \hat{\rho}_1^{1/2}(\hat{\rho}_1^{1/2-2^{-n}}\hat{\rho}_2^{2^{-n}})$ and use the Cauchy-Schwarz inequality again.)

c) Take the limit $n \to \infty$ in order to prove the identity (1).

20. Extremality of density operators II *8 points*

Now, we want to use Eq. (1) in order to see in which sense the density operators of the canonical and grand canonical ensemble maximize the entropy.

a) Let $\hat{\rho}_2$ be the density operator of the canonical ensemble and $\hat{\rho}_1$ be an arbitrary density operator. Define $E \equiv \mathrm{Tr}\hat{\rho}_2\hat{H}$, $E' \equiv \mathrm{Tr}\hat{\rho}_1\hat{H}$, $S \equiv -k_B\mathrm{Tr}\hat{\rho}_2 \ln \hat{\rho}_2$, and $S' \equiv -k_B\mathrm{Tr}\hat{\rho}_1 \ln \hat{\rho}_1$. Show that

$$S \geq S' + \frac{1}{T}(E - E').$$

b) Let $\hat{\rho}_2$ be the density operator of the grand canonical ensemble and $\hat{\rho}_1$ be an arbitrary density operator. Define $E \equiv \mathrm{Tr}\hat{\rho}_2\hat{H}$, $E' \equiv \mathrm{Tr}\hat{\rho}_1\hat{H}$, $N \equiv \mathrm{Tr}\hat{\rho}_2\hat{N}$, $N' \equiv \mathrm{Tr}\hat{\rho}_1\hat{N}$, $S \equiv -k_B\mathrm{Tr}\hat{\rho}_2 \ln \hat{\rho}_2$, and $S' \equiv -k_B\mathrm{Tr}\hat{\rho}_1 \ln \hat{\rho}_1$. Show that

$$S \geq S' + \frac{1}{T}[E - E' - \mu'(N - N')].$$

Department of Physics
The Ohio State University

Prof. R. Bundschuh

Eighth Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important date: Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Mar 2

21. Density operator of a free particle

10 points

A free particle is described by the Hamiltonian $\hat{H} = \hat{\vec{p}}^2/2m$. We assume that the particle is in a cubic box of volume $V = L^3$.

a) Write the canonical density operator in the momentum base $|\vec{k}\rangle$, i.e., calculate $\langle\vec{k}'|\hat{\rho}|\vec{k}\rangle$. When calculating the partition function you may replace the sum by an integral.

b) Write the canonical density operator in the coordinate base $|\vec{r}\rangle$, i.e., calculate $\langle\vec{r}'|\hat{\rho}|\vec{r}\rangle$. You may again replace sums by integrals. (Hint: use $\langle\vec{k}|\vec{r}\rangle = V^{-1/2}\exp(-i\vec{k}\vec{r})$.)

22. Single energy level

10 points

We consider one energy level of a large quantum system as the subsystem which we want to describe while we summarize all the other levels of the system as the particle bath. The single particle energy of the level we picked is ε. Since there is only one level, the state of our subsystem is completely described by the kets $|n\rangle$ where n is the number of particles in our level. Since this number is not fixed, we use the grand canonical ensemble to describe this system.

a) Calculate the probability $p_n = \langle n|\hat{\rho}|n\rangle$ to find n particles in the system as a function of inverse temperature β, the level energy ε, and the fugacity $z = \exp(\beta\mu')$ for a bosonic system.

b) Calculate the average number of particles $\mathrm{Tr}\hat{\rho}\hat{N}$ in the system as a function of inverse temperature β, the level energy ε, and the fugacity $z = \exp(\beta\mu')$ for a bosonic system.

c) Calculate the probability $p_n = \langle n|\hat{\rho}|n\rangle$ to find n particles in the system as a function of inverse temperature β, the level energy ε, and the fugacity $z = \exp(\beta\mu')$ for a fermionic system.

d) Calculate the average number of particles $\mathrm{Tr}\hat{\rho}\hat{N}$ in the system as a function of inverse temperature β, the level energy ε, and the fugacity $z = \exp(\beta\mu')$ for a fermionic system.

23. Two harmonic oscillators *10 points*

Consider two indistinguishable particles inside a harmonic oscillator with frequency ω. The eigenenergies of a single particle in this oscillator are $E_n = \hbar\omega(n + 1/2)$ and we call the normalized eigenvector of the n-th eigenenergy $|n\rangle$.

a) Calculate the canonical partition function of two particles in this oscillator treating it as a classical system with discrete states.

b) Calculate the canonical partition function of two particles in this oscillator assuming that the two particles are bosons.

c) Calculate the canonical partition function of two particles in this oscillator assuming that the two particles are fermions.

Department of Physics
The Ohio State University

Prof. R. Bundschuh

Ninth Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important date: Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Mar 9

24. Two-level bosons

8 points

An ideal Bose-Einstein gas consists of non-interacting bosons of mass m which have an internal degree of freedom which can be described by assuming, that the bosons are two-level atoms. Bosons in the ground state have energy $E_0 = p^2/2m$, while bosons in the excited state have energy $E_1 = p^2/2m + \Delta$, where p is the momentum and Δ is the excitation energy. Assume that $\Delta \gg k_B T$.

a) Find an equation for the Bose-Einstein condensation temperature T_c for this gas of two-level bosons. (Hint: this equation may not be so easy to actually solve since it involves T_c and $\exp(-\beta\Delta) = \exp(-\Delta/k_B T_c)$ at the same time.)

b) Does the existence of the internal degree of freedom raise or lower the condensation temperature?

25. Fermi energy of copper

6 points

Electrons in a piece of copper metal can be assumed to behave like an ideal Fermi-Dirac gas. Copper metal in the solid state has a mass density of $9g/cm^3$. Assume that each copper atom donates one electron to the Fermi-Dirac gas. Assume the system is at $T = 0K$.

a) Compute the Fermi energy ε_F of the electron gas in eV.

b) Compute the Fermi "temperature" $T_F = \varepsilon_F/k_B$.

26. Two-dimensional Fermi gas

10 points

It is experimentally possible to confine electrons to a two-dimensional system. Thus, we want to study the properties of non-interacting spin-1/2 fermions in two dimensions. The fermions have mass m and are confined to a square of area $A = L^2$.

a) Calculate the density of states of this system.

b) Calculate the Fermi energy of the system as a function of the density $n = N/A$ of the fermions. Use this result to replace the fundamental constants in the density of states by the Fermi energy.

c) Show that for low temperatures the chemical potential μ' is independent of temperature.

d) Calculate the internal energy U of the system as a function of the temperature T and the Fermi energy ε_F for low temperatures.

Department of Physics
The Ohio State University

Prof. R. Bundschuh

First Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important dates: Feb 10 10:30am-12:18pm midterm exam,
Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Jan 13

1. Review *10 points*

Let us start by reviewing some of the key concepts from the first statistical mechanics course.

a) What are the three laws of thermodynamics?

b) What is special about the entropy in thermodynamic equilibrium compared to all other possible states of a system?

c) What is a thermodynamic phase transition and what is the difference between a first-order and a continuous phase transition?

d) What is the relation between the entropy of a macroscopic state and the number of microscopic states which correspond to the macroscopic state?

e) What is the probability distribution of the microcanonical ensemble? What physical situation does it correspond to?

2. Harmonic oscillators *10 points*

Let us consider an Einstein solid and look at it from a classical point of view. The Einstein solid picture assumes that atom i of a solid sits at lattice position $\vec{r}_{0,i}$ and can oscillate harmonically around this position. It is described by the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} + \frac{1}{2} m\omega^2 \sum_{i=1}^{N} (\vec{r}_i - \vec{r}_{0,i})^2.$$

a) What shape does the phase space volume with energy less than E, i.e., the volume $H(\vec{x}^N) \leq E$ have?

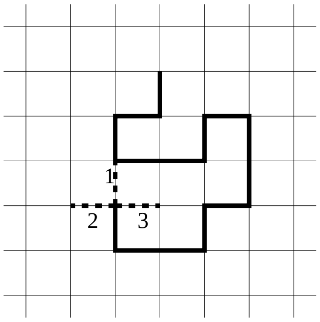
b) Calculate the entropy S of the Einstein solid at a given energy E using classical theory. When you evaluate the constant C_N take into account, that the oscillators have different origins and thus the atoms are distinguishable!

c) In what limit does your result coincide with the quantum mechanical result derived in last quarter's lecture? (You can find last quarter's lecture on the Einstein solid at `http://cannoli.mps.ohio-state.edu/phy846/phy846-14.pdf`)

d) What would the entropy be, if we had a gas of N particles within *the same* harmonic oscillator, i.e., if $\vec{r}_{0,i} = 0$ for all i. Is this entropy an extensive quantity? (Hint: You have to use a different constant C_N.)

3. A polymer on the lattice - microcanonical *10 points*

To appreciate the differences between the microcanonical and the canonical ensemble we want to solve one more problem in the microcanonical ensemble. A simple model for a polymer in two dimensions is that of a path on a square lattice. At every lattice point the polymer can either go straight (option 1 in the figure) or choose between the two directions in a right angle with respect to its current direction (options 2 and 3 in the figure.) Each time it bends in a right angle, it pays a bending energy ϵ. Thus, for a given "shape" of the polymer the total bending energy of the polymer is ϵ times the number of right angle turns. We assume that the starting segment of the polymer is fixed somewhere on the lattice and that the polymer consists of $N+1$ segments. Each possible shape of the polymer is a state of this statistical mechanics system.



a) How many polymer shapes have a total bending energy E where we assume $E = m\epsilon$ with some integer $0 \leq m \leq N$? (Hint: First count how many ways there are to position the m right angles on the polymer of length $N+1$ segments and then take into account that there are 2 possible choices for each right angle, namely left and right.)

b) What is the entropy $S(E, N)$ of this system? Approximate all factorials with the help of Stirling's formula.

c) Calculate the temperature of this system as a function of the total bending energy E and the length N of the polymer.

d) Calculate the energy E of the polymer as a function of the temperature T and of the length N of the polymer.

e) Calculate the heat capacity at constant length C_N as a function of the temperature T and the length N of the polymer.