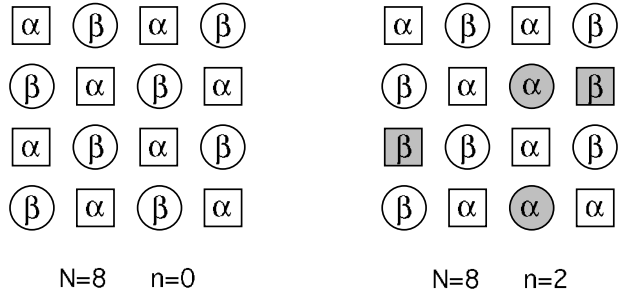


Final Exam

Problem 1 (20 points) Binary Alloy

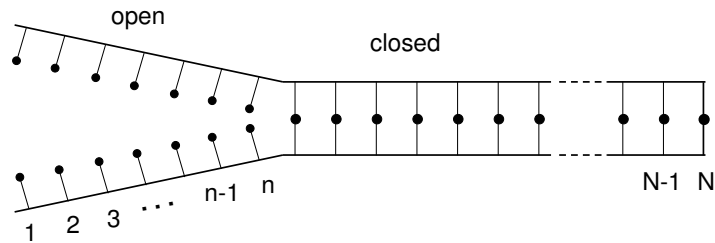


A binary alloy (ZnCu is an example) consists of N α atoms and N β atoms. At low temperatures the system can be modeled as follows. There are N stationary, well defined α -sites which are normally occupied by α atoms and N β -sites normally occupied by β atoms. At $T = 0$ there is perfect order in the system, but at finite temperature n α atoms are displaced to β -sites. (An equal number of β atoms must then be displaced to the vacated α -sites.) The energy of the system associated with the disorder is given by $U = \epsilon n$. If ϵ is a constant, the thermodynamic state of the system is given by a single thermodynamic variable which can be chosen to be either n or U .

To specify one of the many microscopic states of the system consistent with a fixed value of n one must indicate which specific α -sites are occupied by the n β atoms and which specific β -sites are occupied by the n α atoms. For example if $n = 1$ there are N possible sites from which the α atom may be taken, and N possible sites in which it could be placed.

- a) Find the number of different ways of choosing the n α -sites to be vacated and occupied by β atoms.
- b) Find the number of different ways of choosing the n β -sites from which to take the β atoms.
- c) Find the entropy of the system as a function of n .
- d) Find $U(T, N)$.

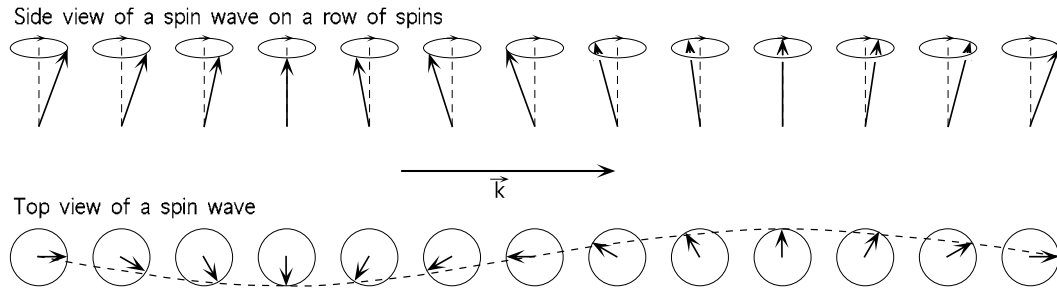
Problem 2 (20 points) DNA Model



A strand of DNA can be modeled as a zipper with links between N base-pairs. Each link has the energy 0 in the closed state and the energy ϵ in the open state. Assume the zipper can only open from one end, so that the n th link can open only if all the links 1, 2, ..., $n-1$ are open. Also assume that N is very large and the system is at temperature T .

- Find the partition function for a single strand $Z_1(T)$ and leave it in the form of a sum which you need not evaluate analytically.
- Find the average number of open links $\langle n \rangle$ at very low temperatures where $kT \ll \epsilon$.
- By converting a sum to an integral find an expression for $Z_1(T)$ where $N\epsilon \gg kT \gg \epsilon$.
- Find the average number of open links $\langle n \rangle$ at high temperatures where $N\epsilon \gg kT \gg \epsilon$.

Problem 3 (20 points) Spin Waves



At low temperatures the coupling between the electronic spins in a solid may cause the moments to align spontaneously in a ferromagnetic state, even in the absence of an applied magnetic field. In the simplest model of ferromagnetism all the spins point in exactly the same direction at $T = 0$. As the temperature is raised, the deviations of the spins from this direction are not localized on single atoms, but rather are spread as correlated disturbances throughout the entire sample. These “normal modes” of the spin system are called spin waves. They are analogous to phonons: spin waves are oscillations in the relative orientations of spins on a lattice; phonons are oscillations in the relative positions of atoms on a lattice.

The spin wave modes are indexed only by their wavevector \vec{k} . For a sample with dimensions L_x , L_y and L_z , the wavevectors allowed by periodic boundary conditions are $\vec{k} = (2\pi/L_x)m\hat{x} + (2\pi/L_y)n\hat{y} + (2\pi/L_z)l\hat{z}$ where m , n and l can take on all positive and negative integer values. Each spin wave mode is represented by a quantum mechanical harmonic oscillator with radian frequency $\omega(\vec{k})$. [The statistical mechanics of a single quantum harmonic oscillator are summarized on the information sheet.]

- What is the density of allowed wavevectors $D(\vec{k})$ such that $D(\vec{k})dk_xdk_ydk_z$ gives the number of allowed wavevectors in the volume $dk_xdk_ydk_z$ around the point \vec{k} in k -space?
- Assume that the dispersion relation for the spin waves is isotropic and quadratic in the wavevector (a good approximation for cubic lattices at low temperatures): $\omega(\vec{k}) = ak^2$ where $k \equiv |\vec{k}|$ and a is a constant. Find an expression for the density of states as a function of frequency $D(\omega)$. Sketch $D(\omega)$.
- Find the spin wave contribution to the heat capacity of the solid $C_V(T, V)$. Leave your answer in terms of a dimensionless integral which you need not evaluate. Since the zero point energy terms do not depend on temperature, you may leave them out from the beginning.
- Does the answer you found in c) exhibit energy gap behavior? If so, explain why; if not, explain why it does not.

Problem 4 (20 points) Graphene

Graphene is a sheet of tightly bound carbon atoms exactly one atomic layer thick. Electrons in the conduction band travel in this sheet as a two-dimensional gas with a unique dispersion relation: it is linear in the magnitude of the wavevector \vec{k} .

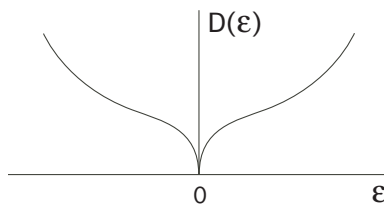
$$\epsilon(\vec{k}) = \hbar v |\vec{k}|$$

For a sample with dimensions L_x by L_y the wavevectors allowed by periodic boundary conditions are $\vec{k} = (2\pi/L_x)m\hat{x} + (2\pi/L_y)n\hat{y}$ where m and n can take on all positive and negative integer values.

- What is the density of allowed wavevectors $D(\vec{k})$ in wavevector space?
- Each electron has a spin degeneracy of 2. Find the density of states in the conduction band as a function of energy, $D_c(\epsilon)$.
- There is also a valence band (where the electrons have negative energies) with a density of states $D_v(\epsilon)$ that is the mirror image of the result you found in b). The two bands just touch; there is no gap. The total density of states is the sum of these two

$$D(\epsilon) = D_c(\epsilon) + D_v(\epsilon) \quad \text{where} \quad D_v(\epsilon) = D_c(-\epsilon)$$

as would be the case in the following illustration.



Make a similar sketch of the total density of states using your result from b).

- At $T = 0$ the valence band is completely full and the conduction band is completely empty. Where is the chemical potential μ at $T = 0$? As T increases, will μ move to higher energies, stay where it is, or move to lower energies? Explain the reason for your answer.
- Find an expression for the internal energy $U(T, A)$ of the electrons, defining $U(T=0, A) = 0$ for the purposes of this problem. Leave your answer in terms of a dimensionless integral. Do not try to evaluate the integral. [Note that it takes twice as much energy to move an electron from $-|\epsilon|$ to $|\epsilon|$ as it does to move it from 0 to $|\epsilon|$.]
- Based on your result in e), what is the exponent n for the temperature in the low temperature constant area heat capacity $C_A(T, A) \propto T^n$ for the electrons in graphene?

Problem 5 (20 points) BEC

The density of states as a function of energy for spinless atoms in three dimensions is given by

$$D(\epsilon) = \frac{V}{(2\pi)^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\epsilon}$$

- a) Derive the general relationship between the temperature T , number density $n \equiv N/V$, and chemical potential μ , for a gas of non-interacting bosons. [The expression for the mean occupation number of any single particle state $\langle n(\epsilon) \rangle$ is given on the information sheet.] Leave your answer in terms of a *dimensionless* integral. It will be helpful to introduce the dimensionless variable $\beta\mu \equiv y$. Your integral will be a function of y : $I(y)$. Do not try to evaluate the integral.
- b) Using the result you just derived, find the relationship between the temperature and density at which Bose-Einstein condensation begins. Again, do not evaluate the integral.

As was pointed out in lecture, the chemical potential, μ , for a Bose gas is negative or zero. It is sometimes *mistakenly* stated that the chemical potential tells us how much the internal energy of a system changes when a particle is added. If true, this would be particularly troubling for a Bose gas since it would say that the internal energy of a Bose gas decreases when a particle is added.

- c) Show, with the help of a Maxwell relation, that the correct expression is

$$\left. \frac{\partial U}{\partial N} \right|_{T,V} = \mu - T \left. \frac{\partial \mu}{\partial T} \right|_{N,V} = \left. \frac{\partial y}{\partial \beta} \right|_{N,V} \quad \text{where } y = \beta\mu,$$

and use this to show that $\partial U / \partial N|_{T,V} = 0$ in the Bose condensed phase.

- d) Now consider temperatures and pressures where there is no condensate. Use the results of part a) to show that $\partial U / \partial N|_{T,V}$ can never be negative for a Bose gas.

PARTIAL DERIVATIVE RELATIONSHIPS

Let x, y, z be quantities satisfying a functional relation $f(x, y, z) = 0$. Let w be a function of any two of x, y, z . Then

$$\begin{aligned}\left(\frac{\partial x}{\partial y}\right)_w \left(\frac{\partial y}{\partial z}\right)_w &= \left(\frac{\partial x}{\partial z}\right)_w \\ \left(\frac{\partial x}{\partial y}\right)_z &= \frac{1}{\left(\frac{\partial y}{\partial x}\right)_z} \\ \left(\frac{\partial x}{\partial y}\right)_z \left(\frac{\partial y}{\partial z}\right)_x \left(\frac{\partial z}{\partial x}\right)_y &= -1\end{aligned}$$

COMBINATORIAL FACTS

There are $K!$ different orderings of K objects. The number of ways of choosing L objects from a set of K objects is

$$\frac{K!}{(K-L)!}$$

if the order in which they are chosen matters, and

$$\frac{K!}{L!(K-L)!}$$

if order does not matter.

STERLING'S APPROXIMATION

When $K \gg 1$

$$\ln K! \approx K \ln K - K \quad \text{or} \quad K! \approx (K/e)^K$$

DERIVATIVE OF A LOG

$$\frac{d}{dx} \ln u(x) = \frac{1}{u(x)} \frac{du(x)}{dx}$$

VOLUME OF AN α DIMENSIONAL SPHERE OF RADIUS R

$$\frac{\pi^{\alpha/2}}{(\alpha/2)!} R^\alpha$$

Work in simple systems

Hydrostatic system	$-PdV$
Surface film	γdA
Linear system	$\mathcal{F}dL$
Dielectric material	$\mathcal{E}d\mathcal{P}$
Magnetic material	HdM

Thermodynamic Potentials when work done on the system is $dW = Xdx$

Energy	U	$dU = TdS + \mu dN + Xdx$
Helmholtz free energy	$F = U - TS$	$dF = -SdT + \mu dN + Xdx$
Gibbs free energy	$G = U - TS - Xx$	$dG = -SdT + \mu dN - xdx$
Enthalpy	$H = U - Xx$	$dH = TdS + \mu dN - xdx$
Thermodynamic potential	$\Phi = F - \mu N$	$d\Phi = -SdT - N d\mu + X dx$

Statistical Mechanics of a Quantum Harmonic Oscillator

$$\begin{aligned}\epsilon(n) &= (n + \frac{1}{2})\hbar\omega & n &= 0, 1, 2, \dots \\ p(n) &= e^{-(n+\frac{1}{2})\hbar\omega/kT} / Z(T) \\ Z(T) &= e^{-\frac{1}{2}\hbar\omega/kT} (1 - e^{-\hbar\omega/kT})^{-1} \\ \langle \epsilon(n) \rangle &= \frac{1}{2}\hbar\omega + \hbar\omega(e^{\hbar\omega/kT} - 1)^{-1}\end{aligned}$$

Mean Occupation Number of Single-Particle Quantum States

$$\langle n(\epsilon, T) \rangle = \frac{1}{e^{(\epsilon-\mu)/k_B T} \pm 1}$$

where the + sign applies to Fermions and the - sign to Bosons

Integrals

$$\begin{aligned}\int e^{ax} dx &= \frac{e^{ax}}{a} \\ \int x e^{ax} dx &= \frac{e^{ax}}{a^2}(ax - 1) \\ \int x^2 e^{ax} dx &= \frac{e^{ax}}{a^3}(a^2x^2 - 2ax + 2) \\ \int \frac{dx}{1+e^x} &= \ln \left[\frac{e^x}{1+e^x} \right]\end{aligned}$$

Definite Integrals

For integer n and m

$$\begin{aligned}\int_0^\infty x^n e^{-x} dx &= n! \\ \int_0^\infty \frac{e^{-x}}{\sqrt{x}} dx &= \sqrt{\pi} \\ (2\pi\sigma^2)^{-1/2} \int_{-\infty}^\infty x^{2n} e^{-x^2/2\sigma^2} dx &= 1 \cdot 3 \cdot 5 \cdots (2n-1) \sigma^{2n} \\ \int_0^\infty x e^{-x^2} dx &= \frac{1}{2} \\ \int_0^1 x^m (1-x)^n dx &= \frac{n!m!}{(m+n+1)!}\end{aligned}$$

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8.044 Statistical Physics I
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