Take-home ‘Midterm’ due on April 17, 2017.

Solve 7 out of 8 problems

The main purpose is to review the topics up to Section 30.
You can send me questions, your drafts for my comments, or come to see me in the morning of M and W, but I ask you not to discuss with each other.

The main purpose of your answers is to show that you have clear understanding of the topics. Therefore, if your ‘level of understanding’ is clear, you need not give all the details.

1. [Response of Brownian particle] You may refer to HW3.
A Brownian particle in 3-space with the friction constant $\zeta$ and mass $m$ is subjected to an external force $F(t)$:

$$m\frac{dv}{dt} = -\zeta v + F(t) + w$$

(Mid.1)

is the (Newton’s) equation of motion, where the noise is mean zero and

$$\langle w(t)w(s)^T \rangle = 2k_B T \zeta \delta(t-s).$$

(Mid.2)

If the initial condition is an equilibrium state, the average velocity at time $t$ must depend on $F(s)$ ($s \in [0,t]$) linearly, because the equation of motion is linear in $F$.\(^1\) Thus we may write, assuming that the force is turned on at $t = 0$,

$$\langle v(t) \rangle = \int_0^t ds \phi(t-s) F(s),$$

(Mid.3)

where $\phi$ is called the (linear) response function.

(1) Let $P(v,t)$ be the distribution function for $v$ at time $t$. Assume that the system is spatially uniform. $P$ is governed by [showing this PDE may give you an extra credit]\(^2\)

$$\frac{\partial}{\partial t} P(v,t) = -\frac{\partial}{\partial v} \left[ \frac{1}{m}(-\zeta v + F)P - \frac{k_B T \zeta}{m^2} \frac{\partial}{\partial v} P \right].$$

(Mid.4)

Confirm that the noise does not destroy the equilibrium state of the system if $F = 0$. That is, show that the equilibrium $P$ is just the Maxwell distribution.

(2) Find the response function, explicitly solving the equation of motion. Confirm that its dimension is just as dictated by dimensional analysis.

(3) Show that

$$\phi(t) I = \beta \langle v(t) v(0)^T \rangle,$$

(Mid.5)

where $I$ is the $d \times d$ unit matrix.

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\(^1\) We say $v(s)$ ($s \in [0,t]$) is a linear functional of $F(s)$ ($s \in [0,t]$).
\(^2\) You can straightforwardly mimic 10.4.
2. [RW without immediate retracing]

Let us consider a lattice random walk on a square lattice (2D of course) whose lattice spacing is 1.

(1) What is the mean-square end-to-end distance \( \langle R \cdot R \rangle \) of the walk of \( N \) steps?

\( \theta \)

(2) Suppose immediate returns (retracing the same lattice bond; red steps in the figure) are forbidden (you should recognize that immediate returns are not at all rare in (1)). What do you expect to happen qualitatively for \( \langle R \rangle \) and \( \langle R \cdot R \rangle \)?

(3) Compute the mean-square end-to-end distance for the random walk without immediate returns (following the steps below; you need not follow them).

(i) Suppose \( a_2 \) makes an angle \( \theta \) with \( a_1 \) as shown in the figure. Let us introduce a rotational matrix \( T(\theta) \) so that we can write \( a_2 = T(\theta)a_1 \). Write down \( T \).

Let \( a_j \) be the \( j \)th step vector and \( a_i \) (\( i > j \)) be the \( i \)th step vector. If \( \theta_k \) is the angle between the \( (k-1) \)th and the \( k \)th step vectors, show that we can write

\[ a_j \cdot a_i = a_j \cdot T(\theta_i) \cdots T(\theta_{j+1})a_j. \] (Mid.6)

Notice that if we average this over all the conformations, we can rewrite

\[ \langle a_j \cdot a_i \rangle = \langle a_1 \cdot T(\theta_{i-j+1}) \cdots T(\theta_2)a_1 \rangle. \] (Mid.7)

You may use this formula.

(ii) Write down \( \langle R \cdot R \rangle \) in terms of \( a_1 \) and \( T(\theta_j) \) (\( j = 2, \cdots, N \)).

(iii) Assuming all the angles are statistically independent, show that

\[ \langle R \cdot R \rangle = N + 2\langle a_1 \cdot \sum_{1 \leq j < i \leq N} (T(\theta))^{i-j}a_1 \rangle. \] (Mid.8)

(iv) Converting the sum over \( i \) and \( j \) to that over \( j \) and \( k = i - j \) (you need not be very careful about \pm 1\), perform the sum in (Mid.8). Assuming the angles take only 0 or \pm \pi/2 with equal probability, compute \( \langle R \cdot R \rangle \). Since \( \langle T(\theta) \rangle \) is a subunitary matrix (its eigenvalues are inside the unit circle), and since we are interested in large \( N \), you may ignore the (high) powers of \( \langle T(\theta) \rangle \).
3. [Violation of the second law]
Suppose there is no mixing entropy. Show that the second law is violated.

4 [Absorption of mixed ideal gas, or convenient partition function]
There is a gas mixture consisting of two distinct atomic species $A$ and $B$. The mixture is an ideal gas and the partial pressure of $X$ is $p_X (X = A$ or $B)$. The gas is in equilibrium with an adsorbing metal surface on which there are adsorption sites. Atom $X$ adsorbed at the site is with energy $-E_X$ on the average relative to the one in the gas phase, where $X = A$ or $B$. Each surface site can accommodate at most one atom. I assume that you know how to calculate the chemical potentials of the atoms, knowing the molecular weights; you can leave the quantum densities as $n_{QX}$; no detailed and explicit calculation is required.
(1) Write down the ‘partition function’ (use the most convenient one) for the single site.
(2) Obtain the average surface concentration $n_X (X = A$ or $B)$ of atoms $A$ and $B$.
(3) Find the maximum concentration $n_A$ obtainable with changing only the partial pressure of $B$. (UIUC Qual F95; not good).

5. [Elementary problem about spin system]
Due to the ligand field the degeneracy of the $d$-orbitals of the chromium ion Cr$^{3+}$ is lifted, and the spin Hamiltonian has the following form

$$H = D(S_z^2 - S(S + 1)/2),$$  \hspace{1cm} (Mid.9)

where $D > 0$ is a constant with $S = 3/2$ (the cation is in the term $^4F_{3/2}$).
(1) Compute the occupation probability of each energy level at temperature $T$ (you may use the standard notation $\beta = 1/k_BT$).
(2) Calculate the entropy.
(3) At high temperatures approximately we have $C = k_B(T_0/T)^2$ with $T_0 = 0.27$ K. Determine $D$ in K. (almost UIUC Qual; boring)

6 [Boson-Fermion mixing]
A thermally insulated rigid container is partitioned into two identical halves of volume $V$ (see the accompanying figure) with a rigid and thermally-insulating wall. The left half contains an ideal fermion gas (spinless, i.e., you may ignore spins) consisting of $N$ particles and the right contains an ideal boson gas.

Initially, both partitions are in equilibrium and have the same pressure $P$. For simplicity,
let us assume that the fermion side is at $T = 0$.

(1) The Fermi energy $\mu(0)$ of the left half is 2.5 eV. Demonstrate that the temperature of the right half containing bosons must be hotter than $10^4$ K. You must demonstrate the inequality $T > 10,000$ K. No handwaving argument is enough (Needed thermodynamic inequalities must be shown). [Hint: think of $P$ with various statistics under the same $T, V, N$ condition.]

(2) The partition is removed suddenly (by, e.g., punctuating), and a new equilibrium uniform state is eventually realized. What is the pressure of the final equilibrium?

7. [Stability]
Let $X$ and $Y$ be extensive thermodynamic variables.

(1) Show

$$\langle \delta X \delta Y \rangle^2 \leq \langle \delta X^2 \rangle \langle \delta Y^2 \rangle. \tag{Mid.10}$$

(2) What is the thermodynamic implication of this natural inequality? In other words, write down the equivalent formula in terms of an appropriate Jacobian. Recognize how mathematically natural the thermodynamic stability conditions are.

(3) What is the generalization of (Mid.10) to the $n$-extensive variable case \{X, X_2, \cdots, X_n\}?

8. [Basic problem for quantum ideal gas: compression under constant internal energy]\(^3\)
In a cylinder with a piston is an ideal gas consisting of $N$ particles, whose initial temperature is $T_i$. The piston is pushed in slowly to halve the volume while removing thermal energy appropriately to keep the internal energy constant. Let $T_f$ be the final temperature.

I. The case of spinless bosons: assume that there is a Bose-Einstein condensate initially.

(1) Find the number of particles $N_0$ in the condensate before compression. You may use the critical temperature $T_c$.

(2) Which is true, $T_f < T_i$, $T_f = T_i$ or $T_f > T_i$?

(3) Does the number of particles in the condensate increase or decrease?

II. The case of ‘spinless’ fermions.

(4) Find the final pressure $P_f$.

(5) Is there a minimum temperature ($> 0$) below which this process becomes impossible?

(6) Which is true, $T_f < T_i$, $T_f = T_i$ or $T_f > T_i$?

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\(^3\)I may have posted the solution somewhere, but in that case you must write your well-digested result.