Statistical Mechanics/Quantum Mechanics
General Exam
January 18, 2008
09:00 - 15:00 in P-121

Answer at most **four** (4) questions from each of the **two** (2) sections for a total of **six** (6) solutions. If you turn in excess solutions, the ones to be graded will be picked at random.

Each answer must be presented separately in an answer book, or on consecutively numbered sheets of paper stapled together. Make sure you clearly indicate who you are, and what is the problem you are answering. Double-check that you include everything you want graded, and nothing else.

Section A — mostly statistical mechanics

A1. A monatomic gas obeys the van der Waals equation, which for a fixed atom number may be cast in the form

$$p = \frac{NkT}{V-b} - \frac{a}{V^2}\,, \tag{1}$$

and has the heat capacity at constant volume $C_V = \frac{3}{2}Nk$. Here $a > 0$ and $b > 0$ are constants, and $V > b$.

(a) Even for a fixed atom number, the heat capacity could still depend on volume. Nevertheless, using thermodynamic identities show that *any* heat capacity compatible with the equation of state (1) must satisfy

$$\left(\frac{\partial C_V}{\partial V}\right)_T = 0\,.$$

(b) Find the entropy of the van der Waals gas, $S(T,V)$, to within an additive constant.

(c) Find the internal energy, $U(T,V)$, to within an additive constant.

(d) What is the final temperature when the gas is adiabatically compressed from (V_1, T_1) to the final volume V_2?

(e) How much work is done in this compression?

A2. In a two-dimensional two-component ($s = \frac{1}{2}$, $g = 2$) ideal Fermi gas the chemical potential μ may be found analytically in closed form as a function of temperature T and (area) density n. Do it!

A3. The collision derivative in the Boltzmann equation is local, acts separately at each position, so that every one-particle distribution function of the form

$$f(\mathbf{r},\mathbf{p}) = e^{-\dfrac{\mathbf{p}^2}{2mkT} + K(\mathbf{r})}$$

zeroes the collision derivative, $\left(\dfrac{\partial f}{\partial t}\right)_c = 0$, even if the "constant" $K(\mathbf{r})$ depends on position. The particles are acted upon by a conservative force, one that satisfies $\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})$. What is the stationary solution to the Boltzmann equation in the presence of the force? Absent any further knowledge about $V(\mathbf{r})$, the solution is formal only; do not worry about the normalization.

A4. Consider a nanosystem in which only two energy levels are relevant to the thermodynamic properties at moderate temperatures. Let us denote these levels by e_0 and e_1 with $e_0 < e_1$. The lower and upper levels contain ω_0 and ω_1 single particle states respectively. In the ground state, the lower level has a single electron while the upper level is empty. If the energy difference is far less than the typical thermal energies at room temperature, then the higher level can have a considerable population and thus influence the thermodynamic properties of the system at room temperature.

a) Show that the heat capacity C at temperature T due to electronic motion in such a system is given by $C = f(\omega, \epsilon, T)$ with $\omega = \omega_1/\omega_0$ and $\epsilon = e_1/k_B$. Here the lower energy level is taken to be zero. Find the function f.

b) Obtain approximations for C in the limits of high and low temperatures. Does C have an extremum as a function of T?

c) For a system that has two such close energy levels with $\epsilon = 174\,\mathrm{K}$, sketch C vs T assuming $\omega_0 = 3$ and $\omega_1 = 2$.

Hint: Do not blindly use Fermi-Dirac type distributions.

Section B — mostly quantum mechanics

B1. Consider the infinite square well potential with the width a:

$$V(x) = \begin{cases} 0, & x \in (0, a)\,, \\ \infty, & \text{otherwise}\,. \end{cases}$$

The eigenstates for this potential are

$$\psi_n(x) \quad = \quad \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x\,,$$

with $n = 1, 2, \ldots$.

Suppose a particle is initially in the ground state ψ_1. If we move the right wall out to $2a$, evaluate the probability to find the particle in the first excited state ($n = 2$) of the expanded well for the following two cases:

(a) We move the wall gradually (adiabatically).

(b) We move the wall suddenly.

B2. An operator associated with an infinitesimal rotation can be written as

$$1 + \delta\phi\, \hat{\mathbf{n}} \cdot (\mathbf{r} \times \nabla)\,, \tag{2}$$

where $\delta\phi$ is the rotation angle and $\hat{\mathbf{n}}$ is the unit vector in the direction of the axis of rotation.

(a) Define the generators L_x, L_y and L_z associated with such rotations using (2). Show that they are Hermitian.

(b) Find the commutators $[L_x, L_z]$ and $[\mathbf{L}^2, L_z]$ using your definitions.

(c) Use the Hermiticity of the generators L_x, L_y, L_z of infinitesimal rotations to show that they preserve the normalization of any wave function $\psi(\mathbf{r})$; i.e., that the normalization is invariant under such rotations.

B3. Consider the operators A and B satisfying $[A, [A, B]] = [B, [A, B]] = 0$.

(a) Show that $[A^m, B] = m\, A^{m-1}[A, B]$ holds for all positive integers m, using mathematical induction.

(b) Using the above, show that $[e^{-\lambda A}, B] = \lambda e^{-\lambda A}[B, A]$ and hence that

$$e^{\lambda A} B e^{-\lambda A} = B - \lambda[B, A]\,.$$

(c) Using a scalar variable λ, write $T(\lambda) = e^{\lambda A}\, e^{\lambda B}$ and show that

$$\frac{dT}{d\lambda} = (A + B + \lambda[A, B])\, T\,.$$

From this, can you deduce whether $e^{\lambda(A+B)}$ and $T(\lambda)$ are equal or not? Why?

B4. Consider a stylized but (with proper interpretation) accurate model for spectroscopic studies involving three states in an atom or molecule. The Hamiltonian is

$$\frac{H_0}{\hbar} = \omega_g |g\rangle\langle g| + \omega_1 |1\rangle\langle 1| + \omega_2 |2\rangle\langle 2| \,,$$

where g stands for the ground state, and 1 and 2 for two excited states.

(a) What is the resonance frequency for a laser coupling to the $g \to 1$ transition?

(b) Suppose now that another laser couples to the $g \to 2$ transition, as per

$$\frac{H'}{\hbar} = \Omega(|g\rangle\langle 2| + |2\rangle\langle g|) \,.$$

The parameter Ω, Rabi frequency, is proportional to the strength of the electric field of the laser; the parameter $\Delta = \omega_2 - \omega_g$, detuning, depends on the tuning of the laser (do not worry how, that is a feature of the model). This second laser shifts the resonance frequency as observed in the $g \to 1$ transition. Find the shift to the lowest nontrivial order in the Rabi frequency Ω.

B5. The electron in a hydrogen atom occupies the combined spin and position state

$$R_{21}\left(\sqrt{\frac{1}{3}}\, Y_1^0 \chi_+ + \sqrt{\frac{2}{3}}\, Y_1^1 \chi_-\right) .$$

(a) Let $J \equiv L + S$ be the total angular momentum. If you measured J^2 and J_z of the electron, what values might you get, and what is the probability of each?

(b) If you measured the position of the electron, what is the probability density for finding it at r, θ, ϕ?

(c) If you measured both the z component of the spin and the distance from the origin, what is the probability density finding the electron with spin up and at radius r?

Useful formulas:

$$\begin{aligned} R_{21} &= \frac{1}{\sqrt{24a^3}}\,\frac{r}{a}\,\exp\left(-\frac{r}{2a}\right) \\ Y_1^0 &= \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta \\ Y_1^1 &= -\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{i\phi} \end{aligned}$$

All integrals are with respect to the usual measure for spherical polar coordinates, $d^3r = r^2 dr\, \sin\theta\, d\theta\, d\phi$.