8.333: Statistical Mechanics I **Final Exam & Solutions** **12/21/05** (9:00am–noon)

Answer all problems, but note that the first parts of each problem are easier than its last parts. Therefore, make sure to proceed to the next problem when you get stuck.

You may find the following information helpful:

Physical Constants

Electron mass	$m_e \approx 9.1 \times 10^{-31}$kg	Proton mass	$m_p \approx 1.7 \times 10^{-27}$kg
Electron Charge	$e \approx 1.6 \times 10^{-19}$C	Planck's constant/2π	$\hbar \approx 1.1 \times 10^{-34}$Js
Speed of light	$c \approx 3.0 \times 10^{8}$ms^{-1}	Stefan's constant	$\sigma \approx 5.7 \times 10^{-8}Wm^{-2}\,{}^\circ$K^{-4}
Boltzmann's constant	$k_B \approx 1.4 \times 10^{-23} JK^{-1}$	Avogadro's number	$N_0 \approx 6.0 \times 10^{23}$mol^{-1}
Gravitational constant	$G \approx 6.7 \times 10^{-11}$Nm^{2}kg^{-2}		

Conversion Factors

$1atm \equiv 1.0 \times 10^5 Nm^{-2}$ $\qquad 1\mathring{A} \equiv 10^{-10}m$ $\qquad 1eV \equiv 1.1 \times 10^4\,{}^\circ K$

Thermodynamics

$dE = TdS + dW$ $\qquad$ For a gas: $dW = -PdV$ $\qquad$ For a film: $dW = \sigma dA$

Mathematical Formulas

$\lim_{x\to 0} \ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} + \mathcal{O}\left(x^4\right)$ $\qquad$ $\lim_{x\to\infty} \ln(1+x) = \ln x + \frac{1}{x} + \mathcal{O}\left(\frac{1}{x^2}\right)$

$\lim_{x\to\infty} \coth x = 1 + 2e^{-2x} + \mathcal{O}\left(e^{-4x}\right)$ $\qquad$ $\lim_{x\to 0} \coth x = \frac{1}{x} + \frac{x}{3} + \mathcal{O}\left(x^2\right)$

$\int_0^\infty dx\; x^n\; e^{-\alpha x} = \frac{n!}{\alpha^{n+1}}$ $\qquad$ $(\frac{1}{2})! = \frac{\sqrt{\pi}}{2}$

$\int_{-\infty}^{\infty} dx \exp\left[-ikx - \frac{x^2}{2\sigma^2}\right] = \sqrt{2\pi\sigma^2} \exp\left[-\frac{\sigma^2 k^2}{2}\right]$ $\qquad$ $\lim_{N\to\infty} \ln N! = N\ln N - N$

$\left\langle e^{-ikx}\right\rangle = \sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} \langle x^n \rangle$ $\qquad$ $\ln\left\langle e^{-ikx}\right\rangle = \sum_{n=1}^{\infty} \frac{(-ik)^n}{n!} \langle x^n \rangle_c$

$f_m^\eta(z) = \frac{1}{(m-1)!}\int_0^\infty dx \frac{x^{m-1}}{z^{-1}e^x - \eta} = \sum_{\alpha=1}^{\infty} \eta^{\alpha+1} \frac{z^\alpha}{\alpha^m}$ $\qquad$ $\frac{df_m^\eta}{dz} = \frac{1}{z} f_{m-1}^\eta$

$\zeta_m \equiv f_m^+(1)$ $\qquad \zeta_{3/2} \approx 2.612 \qquad \zeta_2 = \frac{\pi^2}{6} \qquad \zeta_{5/2} \approx 1.341 \qquad \zeta_3 \approx 1.202 \qquad \zeta_4 = \frac{\pi^4}{90}$

$\lim_{z\to\infty} f_m^-(z) = \frac{(\ln z)^m}{m!}\left[1 + \frac{\pi^2}{6} m(m-1)(\ln z)^{-2} + \cdots\right]$ $\qquad$ $f_m^-(1) = \left(1 - 2^{1-m}\right)\zeta_m$

1. *Graphene* is a single sheet of carbon atoms bonded into a *two dimensional* hexagonal lattice. It can be obtained by exfoliation (repeated peeling) of graphite. The band structure of graphene is such that the single particles excitations behave as relativistic Dirac *fermions*, with a spectrum that at low energies can be approximated by

$$\mathcal{E}_{\pm}(\vec{k}) = \pm\hbar v \left|\vec{k}\right| \quad .$$

There is spin degeneracy of $g = 2$, and $v \approx 10^6 \mathrm{ms}^{-1}$. Recent experiments on unusual transport properties of graphene were reported in *Nature* **438**, 197 (2005). In this problem, you shall calculate the heat capacity of this material.

(a) If at zero temperature all negative energy states are occupied and all positive energy ones are empty, find the chemical potential $\mu(T)$.

(b) Show that the mean excitation energy of this system at finite temperature satisfies

$$E(T) - E(0) = 4A \int \frac{d^2\vec{k}}{(2\pi)^2} \frac{\mathcal{E}_+(\vec{k})}{\exp\left(\beta\mathcal{E}_+(\vec{k})\right) + 1} \quad .$$

(c) Give a closed form answer for the excitation energy by evaluating the above integral.

(d) Calculate the heat capacity, C_V, of such massless Dirac particles.

(e) Explain qualitatively the contribution of phonons (lattice vibrations) to the heat capacity of graphene. The typical sound velocity in graphite is of the order of $2 \times 10^4 \text{ms}^{-1}$. Is the low temperature heat capacity of graphene controlled by phonon or electron contributions?

2. *Quantum Coulomb gas:* Consider a *quantum* system of N positive, and N negative charged relativistic particles in box of volume $V = L^3$. The Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^{2N} c|\vec{p}_i\,| + \sum_{i<j}^{2N} \frac{e_i e_j}{|\vec{r}_i - \vec{r}_j|} \quad ,$$

where $e_i = +e_0$ for $i = 1, \cdots N$, and $e_i = -e_0$ for $i = N+1, \cdots 2N$, denote the charges of the particles; $\{\vec{r}_i\}$ and $\{\vec{p}_i\}$ their coordinates and momenta respectively. While this is too complicated a system to solve, we can nonetheless obtain some exact results.

(a) Write down the Schrödinger equation for the eigenvalues $\varepsilon_n(L)$, and (in coordinate space) eigenfunctions $\Psi_n(\{\vec{r}_i\})$. State the constraints imposed on $\Psi_n(\{\vec{r}_i\})$ if the particles are bosons or fermions?

(b) By a change of scale $\vec{r}_i{}' = \vec{r}_i/L$, show that the eigenvalues satisfy a scaling relation $\varepsilon_n(L) = \varepsilon_n(1)/L$.

(c) Using the formal expression for the partition function $Z(N, V, T)$, in terms of the eigenvalues $\{\varepsilon_n(L)\}$, show that Z does not depend on T and V separately, but only on a specific scaling combination of them.

(d) Relate the energy E, and pressure P of the gas to variations of the partition function. Prove the exact result $E = 3PV$.

(e) The Coulomb interaction between charges in in d-dimensional space falls off with separation as $e_i e_j / |\vec{r}_i - \vec{r}_j|^{d-2}$. (In $d = 2$ there is a logarithmic interaction.) In what dimension d can you construct an exact relation between E and P for *non-relativistic* particles (kinetic energy $\sum_i \vec{p}_i^{\,2}/2m$)? What is the corresponding exact relation between energy and pressure?

(f) Why are the above 'exact' scaling laws not expected to hold in dense (liquid or solid) Coulomb mixtures?

3. *Non-interacting Fermions:* Consider a grand canonical ensemble of non-interacting *fermions* with chemical potential μ. The one–particle states are labelled by a wavevector $\vec{k}$, and have energies $\mathcal{E}(\vec{k})$.

(a) What is the joint probability $P(\{n_{\vec{k}}\})$, of finding a set of occupation numbers $\{n_{\vec{k}}\}$, of the one–particle states?

(b) Express your answer to part (a) in terms of the average occupation numbers $\left\{\langle n_{\vec{k}}\rangle_{-}\right\}$.

(c) A random variable has a set of ℓ discrete outcomes with probabilities p_n, where $n = 1, 2, \cdots, \ell$. What is the entropy of this probability distribution? What is the maximum possible entropy?

(d) Calculate the entropy of the probability distribution for fermion occupation numbers in part (b), and comment on its zero temperature limit.

(e) Calculate the variance of the total number of particles $\left\langle N^2 \right\rangle_c$, and comment on its zero temperature behavior.

(f) The number fluctuations of a gas is related to its compressibility κ_T, and number density $n = N/V$, by

$$\left\langle N^2 \right\rangle_c = N n k_B T \kappa_T \quad .$$

Give a *numerical estimate* of the compressibility of the fermi gas in a metal at $T = 0$ in units of $\mathring{A}^3 eV^{-1}$.