Review Problems

The third in-class test will take place on Wednesday 11/28/07 from

2:30 to 4:00 pm. There will be a recitation with test review on Monday 11/26/07.

The test is 'closed book,' but if you wish you may bring a one-sided sheet of formulas. The test will be composed entirely from a subset of the following problems. Thus if you are familiar and comfortable with these problems, there will be no surprises!

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 const./2 π	$\hbar\approx 1.1\times 10^{-34}Js^{-1}$
Speed of light	$c\approx 3.0\times 10^8 m s^{-1}$	Stefan's const.	$\sigma\approx 5.7\times 10^{-8}Wm^{-2}K^{-4}$
Boltzmann's const.	$k_B \approx 1.4 \times 10^{-23} J K^{-1}$	Avogadro's number	$N_0 \approx 6.0 \times 10^{23} mol^{-1}$

Conversion Factors

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

Mathematical Formulas

$$\int_{0}^{\infty} dx \ x^{n} \ e^{-\alpha x} = \frac{n!}{\alpha^{n+1}} \qquad \left(\frac{1}{2}\right)! = \frac{\sqrt{\pi}}{2}$$

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

$$\langle e^{-ikx} \rangle = \sum_{n=0}^{\infty} \frac{(-ik)^{n}}{n!} \langle x^{n} \rangle \qquad \ln \langle e^{-ikx} \rangle = \sum_{n=1}^{\infty} \frac{(-ik)^{n}}{n!} \langle x^{n} \rangle_{c}$$

$$\cosh(x) = 1 + \frac{x^{2}}{2!} + \frac{x^{4}}{4!} + \cdots \qquad \sinh(x) = x + \frac{x^{3}}{3!} + \frac{x^{5}}{5!} + \cdots$$

Surface area of a unit sphere in d dimensions

 $S_d = \frac{2\pi^{d/2}}{(d/2-1)!}$

1. Debye-Hückel theory and ring diagrams: The virial expansion gives the gas pressure as an analytic expansion in the density n = N/V. Long range interactions can result in non-analytic corrections to the ideal gas equation of state. A classic example is the Coulomb interaction in plasmas, whose treatment by Debye-Hückel theory is equivalent to summing all the ring diagrams in a cumulant expansion.

For simplicity consider a gas of N electrons moving in a uniform background of positive charge density Ne/V to ensure overall charge neutrality. The Coulomb interaction takes the form

$$\mathcal{U}_Q = \sum_{i < j} \mathcal{V}(\vec{q_i} - \vec{q_j}), \quad \text{with} \quad \mathcal{V}(\vec{q}) = \frac{e^2}{4\pi |\vec{q}|} - c.$$

The constant c results from the background and ensures that the first order correction vanishes, i.e. $\int d^3 \vec{q} \, \mathcal{V}(\vec{q}) = 0.$

(a) Show that the Fourier transform of $\mathcal{V}(\vec{q})$ takes the form

$$\tilde{\mathcal{V}}\left(\vec{\omega}\right) = \begin{cases} e^2/\omega^2 & \text{for } \vec{\omega} \neq 0\\ 0 & \text{for } \vec{\omega} = 0 \end{cases}.$$

(b) In the cumulant expansion for $\left\langle \mathcal{U}_{Q}^{\ell} \right\rangle_{c}^{0}$, we shall retain only the diagrams forming a ring; which are proportional to

$$R_{\ell} = \int \frac{d^3 \vec{q_1}}{V} \cdots \frac{d^3 \vec{q_{\ell}}}{V} \mathcal{V}(\vec{q_1} - \vec{q_2}) \mathcal{V}(\vec{q_2} - \vec{q_3}) \cdots \mathcal{V}(\vec{q_{\ell}} - \vec{q_1}).$$

Use properties of Fourier transforms to show that

$$R_{\ell} = \frac{1}{V^{\ell-1}} \int \frac{d^3 \vec{\omega}}{(2\pi)^3} \, \widetilde{\mathcal{V}}(\vec{\omega})^{\ell}.$$

(c) Show that the number of ring graphs generated in $\left\langle \mathcal{U}_{Q}^{\ell} \right\rangle_{c}^{0}$ is

$$S_{\ell} = \frac{N!}{(N-\ell)!} \times \frac{(\ell-1)!}{2} \approx \frac{(\ell-1)!}{2} N^{\ell}.$$

(d) Show that the contribution of the ring diagrams can be summed as

$$\ln Z_{\rm rings} = \ln Z_0 + \sum_{\ell=2}^{\infty} \frac{(-\beta)^{\ell}}{\ell!} S_{\ell} R_{\ell}$$
$$\approx \ln Z_0 + \frac{V}{2} \int_0^{\infty} \frac{4\pi\omega^2 d\omega}{(2\pi)^3} \left[\left(\frac{\kappa}{\omega}\right)^2 - \ln\left(1 + \frac{\kappa^2}{\omega^2}\right) \right],$$

where $\kappa = \sqrt{\beta e^2 N/V}$ is the inverse Debye screening length. (*Hint:* Use $\ln(1+x) = -\sum_{\ell=1}^{\infty} (-x)^{\ell}/\ell$.)

(e) The integral in the previous part can be simplified by changing variables to $x = \kappa/\omega$, and performing integration by parts. Show that the final result is

$$\ln Z_{\rm rings} = \ln Z_0 + \frac{V}{12\pi} \,\kappa^3$$

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(f) Calculate the correction to pressure from the above ring diagrams.

(g) We can introduce an effective potential $\overline{V}(\vec{q} - \vec{q'})$ between two particles by integrating over the coordinates of all the other particles. This is equivalent to an expectation value that can be calculated perturbatively in a cumulant expansion. If we include only the loop-less diagrams (the analog of the rings) between the particles, we have

$$\overline{V}(\vec{q} - \vec{q}') = V(\vec{q} - \vec{q}') + \sum_{\ell=1}^{\infty} (-\beta N)^{\ell} \int \frac{d^3 \vec{q_1}}{V} \cdots \frac{d^3 \vec{q_\ell}}{V} \mathcal{V}(\vec{q} - \vec{q_1}) \mathcal{V}(\vec{q_1} - \vec{q_2}) \cdots \mathcal{V}(\vec{q_\ell} - \vec{q}').$$

Show that this sum leads to the screened Coulomb interaction $\overline{V}(\vec{q}) = \exp(-\kappa |\vec{q}|)/(4\pi |\vec{q}|)$.

2. Virial coefficients: Consider a gas of particles in *d*-dimensional space interacting through a pair-wise central potential, $\mathcal{V}(r)$, where

$$\mathcal{V}(r) = \begin{cases} +\infty & \text{for } 0 < r < a, \\ -\varepsilon & \text{for } a < r < b, \\ 0 & \text{for } b < r < \infty. \end{cases}$$

(a) Calculate the second virial coefficient $B_2(T)$, and comment on its high and low temperature behaviors.

(b) Calculate the first correction to isothermal compressibility

$$\kappa_T = -\frac{1}{V} \left. \frac{\partial V}{\partial P} \right|_{T,N}$$

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(c) In the high temperature limit, reorganize the equation of state into the van der Waals form, and identify the van der Waals parameters.

(d) For b = a (a hard sphere), and d = 1, calculate the third virial coefficient $B_3(T)$.

3. Dieterici's equation: A gas obeys Dieterici's equation of state:

$$P(v-b) = k_B T \exp\left(-\frac{a}{k_B T v}\right),$$

where v = V/N.

(a) Find the ratio Pv/k_BT at the critical point.

- (b) Calculate the isothermal compressibility κ_T for $v = v_c$ as a function of $T T_c$.
- (c) On the critical isotherm expand the pressure to the lowest non-zero order in $(v v_c)$. *******

4. Two dimensional Coulomb gas: Consider a classical mixture of N positive, and N negative charged particles in a two dimensional box of area $A = L \times L$. The Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^{2N} \frac{\vec{p_i}^2}{2m} - \sum_{i< j}^{2N} c_i c_j \ln |\vec{q_i} - \vec{q_j}| \quad ,$$

where $c_i = +c_0$ for $i = 1, \dots, N$, and $c_i = -c_0$ for $i = N + 1, \dots, 2N$, denote the charges of the particles; $\{\vec{q}_i\}$ and $\{\vec{p}_i\}$ their coordinates and momenta respectively.

(a) Note that in the interaction term each pair appears only once, and that there is no self interaction i = j. How many pairs have repulsive interactions, and how many have attractive interactions?

(b) Write down the expression for the partition function Z(N, T, A) in terms of integrals over $\{\vec{q}_i\}$ and $\{\vec{p}_i\}$. Perform the integrals over the momenta, and rewrite the contribution of the coordinates as a product involving powers of $\{\vec{q}_i\}$, using the identity $e^{\ln x} = x$.

(c) Although it is not possible to perform the integrals over $\{\vec{q}_i\}$ exactly, the dependence of Z on A can be obtained by the simple rescaling of coordinates, $\vec{q}_i' = \vec{q}_i/L$. Use the results in parts (a) and (b) to show that $Z \propto A^{2N-\beta c_0^2 N/2}$.

(d) Calculate the two dimensional pressure of this gas, and comment on its behavior at high and low temperatures.

(e) The unphysical behavior at low temperatures is avoided by adding a hard-core which prevents the coordinates of any two particles from coming closer than a distance a. The appearance of two length scales a and L, makes the scaling analysis of part (c) questionable. By examining the partition function for N = 1, obtain an estimate for the temperature T_c at which the short distance scale a becomes important in calculating the partition function, invalidating the result of the previous part. What are the phases of this system at low and high temperatures?

5. Exact solutions for a one dimensional gas: In statistical mechanics, there are very few systems of interacting particles that can be solved *exactly*. Such exact solutions are very important as they provide a check for the reliability of various approximations. A one dimensional gas with short-range interactions is one such solvable case.

(a) Show that for a potential with a hard core that screens the interactions from further neighbors, the Hamiltonian for N particles can be written as

$$\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=2}^{N} \mathcal{V}(x_i - x_{i-1}).$$

The (indistinguishable) particles are labelled with coordinates $\{x_i\}$ such that

$$0 \le x_1 \le x_2 \le \dots \le x_N \le L,$$

where L is the length of the box confining the particles.

(b) Write the expression for the partition function Z(T, N, L). Change variables to $\delta_1 = x_1, \delta_2 = x_2 - x_1, \dots, \delta_N = x_N - x_{N-1}$, and carefully indicate the allowed ranges of integration and the constraints.

(c) Consider the Gibbs partition function obtained from the Laplace transformation

$$\mathcal{Z}(T, N, P) = \int_0^\infty dL \exp(-\beta PL) Z(T, N, L),$$

and by extremizing the integrand find the standard formula for P in the canonical ensemble.

(d) Change variables from L to $\delta_{N+1} = L - \sum_{i=1}^{N} \delta_i$, and find the expression for $\mathcal{Z}(T, N, P)$ as a product over one-dimensional integrals over each δ_i .

(e) At a fixed pressure P, find expressions for the mean length L(T, N, P), and the density n = N/L(T, N, P) (involving ratios of integrals which should be easy to interpret).

Since the expression for n(T, P) in part (e) is continuous and non-singular for any choice of potential, there is in fact no condensation transition for the one-dimensional gas. By contrast, the approximate van der Waals equation (or the mean-field treatment) incorrectly predicts such a transition.

(f) For a hard sphere gas, with minimum separation a between particles, calculate the equation of state P(T, n). Compare the excluded volume factor with the approximate result obtained in earlier problems, and also obtain the general virial coefficient $B_{\ell}(T)$.

6. One dimensional chain: A chain of N+1 particles of mass m is connected by N massless springs of spring constant K and relaxed length a. The first and last particles are held

fixed at the equilibrium separation of Na. Let us denote the longitudinal displacements of the particles from their equilibrium positions by $\{u_i\}$, with $u_0 = u_N = 0$ since the end particles are fixed. The Hamiltonian governing $\{u_i\}$, and the conjugate momenta $\{p_i\}$, is

$$\mathcal{H} = \sum_{i=1}^{N-1} \frac{p_i^2}{2m} + \frac{K}{2} \left[u_1^2 + \sum_{i=1}^{N-2} \left(u_{i+1} - u_i \right)^2 + u_{N-1}^2 \right].$$

(a) Using the appropriate (sine) Fourier transforms, find the normal modes $\{\tilde{u}_k\}$, and the corresponding frequencies $\{\omega_k\}$.

(b) Express the Hamiltonian in terms of the amplitudes of normal modes $\{\tilde{u}_k\}$, and evaluate the *classical* partition function. (You may integrate the $\{u_i\}$ from $-\infty$ to $+\infty$).

(c) First evaluate $\langle |\tilde{u}_k|^2 \rangle$, and use the result to calculate $\langle u_i^2 \rangle$. Plot the resulting squared displacement of each particle as a function of its equilibrium position.

(d) How are the results modified if only the first particle is fixed $(u_0 = 0)$, while the other end is free $(u_N \neq 0)$? (Note that this is a much simpler problem as the partition function can be evaluated by changing variables to the N - 1 spring extensions.)

7. Black hole thermodynamics: According to Bekenstein and Hawking, the entropy of a black hole is proportional to its area A, and given by

$$S = \frac{k_B c^3}{4G\hbar} A$$

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(a) Calculate the escape velocity at a radius R from a mass M using classical mechanics. Find the relationship between the radius and mass of a black hole by setting this escape velocity to the speed of light c. (Relativistic calculations do not modify this result which was originally obtained by Laplace.)

(b) Does entropy increase or decrease when two black holes collapse into one? What is the entropy change for the universe (in equivalent number of bits of information), when two solar mass black holes $(M_{\odot} \approx 2 \times 10^{30} kg)$ coalesce?

(c) The internal energy of the black hole is given by the Einstein relation, $E = Mc^2$. Find the temperature of the black hole in terms of its mass.

(d) A "black hole" actually emits thermal radiation due to pair creation processes on its event horizon. Find the rate of energy loss due to such radiation.

(e) Find the amount of time it takes an isolated black hole to evaporate. How long is this time for a black hole of solar mass?

(f) What is the mass of a black hole that is in thermal equilibrium with the current cosmic background radiation at T = 2.7K?

(g) Consider a spherical volume of space of radius R. According to the recently formulated *Holographic Principle* there is a maximum to the amount of entropy that this volume of space can have, independent of its contents! What is this maximal entropy?

8. Quantum harmonic oscillator: Consider a single harmonic oscillator with the Hamiltonian

$$\mathcal{H} = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}, \quad \text{with} \quad p = \frac{\hbar}{i} \frac{d}{dq}$$

(a) Find the partition function Z, at a temperature T, and calculate the energy $\langle \mathcal{H} \rangle$.

(b) Write down the formal expression for the canonical density matrix ρ in terms of the eigenstates ($\{|n\rangle\}$), and energy levels ($\{\epsilon_n\}$) of \mathcal{H} .

(c) Show that for a general operator A(x),

$$\frac{\partial}{\partial x} \exp\left[A(x)\right] \neq \frac{\partial A}{\partial x} \exp\left[A(x)\right], \quad \text{unless} \quad \left[A, \frac{\partial A}{\partial x}\right] = 0,$$

while in all cases

$$\frac{\partial}{\partial x} \operatorname{tr} \left\{ \exp\left[A(x)\right] \right\} = \operatorname{tr} \left\{ \frac{\partial A}{\partial x} \exp\left[A(x)\right] \right\}.$$

(d) Note that the partition function calculated in part (a) does not depend on the mass m, i.e. $\partial Z/\partial m = 0$. Use this information, along with the result in part (c), to show that

$$\left\langle \frac{p^2}{2m} \right\rangle = \left\langle \frac{m\omega^2 q^2}{2} \right\rangle.$$

(e) Using the results in parts (d) and (a), or otherwise, calculate $\langle q^2 \rangle$. How are the results in Problem #6 modified at low temperatures by inclusion of quantum mechanical effects.

(f) In a coordinate representation, calculate $\langle q'|\rho|q\rangle$ in the high temperature limit. One approach is to use the result

$$\exp(\beta A)\exp(\beta B) = \exp\left[\beta(A+B) + \beta^2[A,B]/2 + \mathcal{O}(\beta^3)\right].$$

(g) At low temperatures, ρ is dominated by low energy states. Use the ground state wave-function to evaluate the limiting behavior of $\langle q' | \rho | q \rangle$ as $T \to 0$.

(h) Calculate the exact expression for $\langle q'|\rho|q\rangle$.

9. Relativistic 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 $i = 1, \dots, N$, and $e_i = -e_0$ for $i = N + 1, \dots, 2N$, 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?

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10. The virial theorem is a consequence of the invariance of the phase space for a system of N (classical or quantum) particles under canonical transformations, such as a change of scale. In the following, consider N particles with coordinates $\{\vec{q}_i\}$, and conjugate momenta $\{\vec{p}_i\}$ (with $i = 1, \dots, N$), and subject to a Hamiltonian $\mathcal{H}(\{\vec{p}_i\}, \{\vec{q}_i\})$.

(a) Classical version: Write down the expression for the classical partition function, $Z \equiv Z[\mathcal{H}]$. Show that it is invariant under the rescaling $\vec{q_1} \rightarrow \lambda \vec{q_1}$, $\vec{p_1} \rightarrow \vec{p_1}/\lambda$ of a pair of conjugate variables, i.e. $Z[\mathcal{H}_{\lambda}]$ is independent of λ , where \mathcal{H}_{λ} is the Hamiltonian obtained after the above rescaling.

(b) Quantum mechanical version: Write down the expression for the quantum partition function. Show that it is also invariant under the rescalings $\vec{q_1} \rightarrow \lambda \vec{q_1}$, $\vec{p_1} \rightarrow \vec{p_1}/\lambda$, where $\vec{p_i}$ and $\vec{q_i}$ are now quantum mechanical operators. (Hint: start with the time-independent Schrödinger equation.)

(c) Now assume a Hamiltonian of the form

$$\mathcal{H} = \sum_{i} \frac{\vec{p_i}^2}{2m} + V\left(\{\vec{q_i}\}\right)$$

Use the result that $Z[\mathcal{H}_{\lambda}]$ is independent of λ to prove the *virial* relation

$$\left\langle \frac{\vec{p_1}^2}{m} \right\rangle = \left\langle \frac{\partial V}{\partial \vec{q_1}} \cdot \vec{q_1} \right\rangle,$$

where the brackets denote thermal averages.

(d) The above relation is sometimes used to estimate the mass of distant galaxies. The stars on the outer boundary of the G-8.333 galaxy have been measured to move with velocity $v \approx 200$ km/s. Give a numerical estimate of the ratio of the G-8.333's mass to its size.

8.333 Statistical Mechanics I: Statistical Mechanics of Particles Fall 2013

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