PC5202, Assignment 2

Due Thursday, 13 Feb 20

1. The classical Poisson bracket is defined as

$$(A,B) = \sum_j \left(\frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j} - \frac{\partial B}{\partial q_j}\frac{\partial A}{\partial p_j} \right),$$

while the quantum mechanical version is defined by commutator

$$(\hat{A},\hat{B}) = \frac{\hat{A}\hat{B} - \hat{B}\hat{A}}{i\hbar} = \frac{1}{i\hbar}[\hat{A},\hat{B}].$$

Note that $(q_j, p_k) = \delta_{jk}$ for coordinates and conjugate momenta both in classical and quantum mechanics. Here δ_{jk} is the Kronecker delta. Show that the Poisson brackets have the following properties valid in both classical and quantum mechanics:

(1) anti-symmetry: $(A,B) = -(B,A)$

(2) linearity: $(A+B,C) = (A,C) + (B,C)$

$(\lambda A, B) = \lambda(A,B)$

where λ is a constant.

(3) Leibniz rule: $(AB,C) = A(B,C) + (A,C)B$

(4) Jacob identity: $\big((A,B),C\big) + \big((B,C),A\big) + \big((C,A),B\big) = 0$

It may require a lot of writing. Please try to be brief.

2. Continue from the first problem above, show that the canonical relation (Poisson bracket in classical mechanics and commutator in quantum mechanics), $(q_j, p_k) = \delta_{jk}$, is invariant with respect to the dynamics, i.e., it is the same whether p and q are at time t = 0 or t > 0. Show this explicitly, (a) for classical mechanics, let $A = Q_j(q,p,t)$, and $B = P_k(q,p,t)$, where Q and P are the solutions of the Hamiltonian equations of motion, with initial condition q and p at time t=0, compute the Poisson bracket (A, B) with respect to variables q,p. (b) For the quantum case, let $\hat{A}$ and $\hat{B}$ be the Heisenberg operators of positions and momenta, i.e., e.g., $Q = U(0,t)qU(t,0)$, where U is the unitary evolution operator, and compute the commutator. (c) Argue or demonstrate explicitly that the conclusion is false if Q and P are at different times.

3. Consider the classical ideal gas system of N point particles with the Hamiltonian

$$H = \sum_{j=1}^{3N} \frac{p_j^2}{2m} + V(q_1, q_2, \ldots, q_{3N}).$$

The effect of the potential energy V is to confine the particles in a box of volume $V = L^3$, and to establish equilibrium. It is treated as 0 otherwise. Study the ideal gas in three different ensembles: micro-canonical, canonical, and grand-canonical. That is, compute the micro-canonical number of states $\Omega(U,V,N)$, the canonical partition function $Z(T,V,N)$, and grand-canonical partition function $\Xi(T,V,\mu)$. Differentiate with respect to appropriate arguments of the fundamental thermodynamic relations [micro-canonical entropy $S(U,V,N)$, the Helmholtz free energy $F(T,V,N)$ in canonical ensemble, and grand potential $\Psi(T,V,\mu)$] to get the equations of states: (1) internal energy U as a function of temperature T, (2) the ideal gas law $PV=Nk_BT$, and (3) the chemical potential μ, or (4) average number of particle $\langle N \rangle$ in the grand-canonical case. Show that the three ensembles give consistent (identical) results for all the quantities calculated in the thermodynamic limit.

Use as known the integrals given in the tutorial problems in the next page. Try to be complete and answer all the questions that have been asked.

Tutorial 2

4. Prove the following mathematical results:

(1) Stirling's formula $\ln n! = n\ln n - n + O(\ln n)$.

(2) Gaussian integral $\int_{-\infty}^{+\infty} e^{-\frac{1}{2}x^2} dx = \sqrt{2\pi}$.

(3) Volume of n-dimensional hypersphere $\int_{x_1^2+x_2^2+\cdots x_n^2 \le 1} dx_1 dx_2 \cdots dx_n = \dfrac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)}$.

The Γ-function is defined by $\Gamma(x+1) = x! = \int_0^\infty t^x e^{-t} dt$.

5. Show that (Yvon's theorem)

$$\left\langle \left(H, B(t)\right) A \right\rangle = k_B T \left\langle \left(A, B(t)\right) \right\rangle$$

where A=A(p,q) and similar for B are arbitrary classical dynamic variables which are zero outside a bounded region in phase space. (A, B) standards for Poisson bracket, and the average < … > is with respect to the canonical distribution. The time dependence means that $B(t) = B(p,q,t) = e^{t(.,H)} B(p,q)$. Do we have a quantum-statistical mechanics analog of this identity?

6. We discuss the generalized Virial theorem and equipartition theorem. Consider an s-degree classical Hamiltonian with an arbitrary potential energy function,

$$H = \sum_{j=1}^{s} \frac{p_j^2}{2m_j} + V(q_{1,} q_2, \cdots, q_s).$$

Show that

$$k_B T = \langle u \cdot \nabla H \rangle$$

where the average $\langle \cdots \rangle$ is over the microcanonical ensemble. u is a 2s-dimensional vector of arbitrary functions of $(q_1, q_2, \cdots, q_s, p_1, p_2, \cdots, p_s)$, such that $\nabla \cdot u = 1$, $\nabla = (\frac{\partial}{\partial q_1}, \frac{\partial}{\partial q_2}, \cdots, \frac{\partial}{\partial q_s}, \frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2}, \cdots, \frac{\partial}{\partial p_s})$. Two important special cases are the equip-partition theorem and virial theorem:

$$k_B T = \left\langle \frac{p_j^2}{m_j} \right\rangle, \quad k_B T = \left\langle q_j \frac{\partial H}{\partial q_j} \right\rangle.$$