Statistical Mechanics

PHYS 508 Spring 2015

Problem Assignment # 5

due 03-06-15

1. **Density matrix** (9 points)

   Consider a free particle of mass m in a cube of volume L^3. Assume periodic boundary conditions for the wave function: $\psi(x+L,y,z) = \psi(x,y+L,z) = \psi(x,y,z+L) = \psi(x,y,z)$.

   (a) Determine the canonical density matrix

   $$\hat{\rho} = \frac{1}{Z}\exp(-\beta\hat{H})$$

   in real space representation (i.e., determine the matrix elements $\langle\vec{x}|\hat{\rho}|\vec{y}\rangle$).

   (b) Show that for $L\to\infty$, the result approaches

   $$\langle\vec{x}|\hat{\rho}|\vec{y}\rangle = \frac{1}{Z}\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2}\exp\left[-\frac{m}{2\beta\hbar^2}(\vec{x}-\vec{y})^2\right] \quad .$$

2. **The harmonic oscillator revisited** (20 points)

   Consider a 1-d harmonic oscillator with Hamiltonian

   $$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2$$

   that is in contact with a heat bath.

   (a) Determine the distribution function $\rho(q)$ for the coordinate q of a classical oscillator (i.e., the probability density for finding the oscillator at position q).

   (b) The same a part **a**, but for a quantum mechanical oscillator.
   hint: (i) From QM, we know that the operator $\hat{n}$ for the observable 'particle density', whose expectation value yields the probability density for finding the particle at point q is, in real space representation, $\langle x|\hat{n}|y\rangle = \delta(x-y)\delta(x-q)$.
   (ii) Use the expressions for $(d/dx)\psi_n(x)$ and $x\ \psi_n(x)$, with $\psi_n(x)$ the oscillator energy eigenfunctions, to derive a differential equation for $\rho(q)$.

   (c) Also determine the distribution function for the momentum in the quantum mechanical case, and discuss all of your results, in particular the limits $\hbar\omega << k_BT$ and $\hbar\omega >> k_BT$.

   (d) Find the canonical density matrix in real space representation.
   hint: (i) For the Hermite polynomials, use the following integral representation:

   $$H_n(x) = (-1)^n e^{x^2}\left(\frac{d}{dx}\right)^n e^{-x^2} = \frac{e^{x^2}}{\sqrt{\pi}}\int_{-\infty}^{\infty} du\ (-2iu)^n e^{-u^2+2ixu} \quad .$$

   (ii) The general Gaussian integral

   $$I(A,b) = \int \Pi_{i=1}^n dx_i\ \exp\left(-\frac{1}{2}\sum_{i,j=1}^n x_i A_{ij} x_j + \sum_{i=1}^n b_i x_i\right)$$

with A a positive definite, real symmetric matrix, can be performed by diagonalizing A. The result is

$$I(A,b) = (2\pi)^{n/2} (\det A)^{-1/2} \exp\left(\frac{1}{2} \sum_{i,j=1}^{n} b_i (A^{-1})_{ij} b_j \right) \quad .$$