Mathematical Physics - PHY307 Fall 2010

Prof. D. Garanin Assignment 4

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1. Calculate the power series

$$\sum_{n=1}^{\infty} \frac{n!}{(2n)!} x^n$$

using Mathematica and plot the result ($x < 0$ also included). Expand the resulting function in Taylor series at $x = 0$ and $x = \pm\infty$. What is the behavior of this function at large positive and negative x?

2. Quantum rotational energy levels of a symmetric molecule are given by

$$E_l = \frac{\hbar^2 l(l+1)}{2I}, \qquad l = 0, 1, 2, \ldots,$$

where I is the moment of inertia of the molecule. The degeneracy of these states is $(2l+1)^2$. Calculate the partition function of these molecules at temperature T

$$Z = \sum_{l=0}^{\infty} (2l+1)^2 \exp\left(-\frac{E_l}{k_B T}\right).$$

Is there an analytical result for Z? Calculate the internal energy of the gas

$$U = \frac{1}{Z} \sum_{l=0}^{\infty} (2l+1)^2 E_l \exp\left(-\frac{E_l}{k_B T}\right)$$

and the heat capacity

$$C = \frac{dU}{dT}.$$

Plot Z, U, and C vs T. For numerical calculations and plotting, set $I = 1/2$ and $\hbar = k_B = 1$.

3. Calculate the Madelung constant of a three-dimensional ionic lattice with alternating charges (generalize the consideration in the lecture notes for $3d$). Provide both the straightforward solution and the intelligent solution assigning coefficients <1 in the sum to the atoms at the borders of the summation range (faces, edges, corners). These coefficients can be found in the German Wikipedia: http://de.wikipedia.org/wiki/Madelung-Konstante.