Homework Assignment Number Eleven Assignment

Problem 1.
Consider the normal distribution

$$f(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

This function does not have an analytical integral.
For the standard normal distribution, where the mean is zero and the standard deviation is one, evaluate the integral from x = -2.0 to 1.0, i.e. $p(-2.0 \le x \le 1.0)$, using

(a) the trapezoidal method with 1 interval.
(b) the trapezoidal method with 10 intervals.
(c) the trapezoidal method with 100 intervals.
(d) the trapezoidal method with 1000 intervals.
(e) the Simpson's Second Order method with 100 intervals.
(f) the Simpson's Second Order method with 1000 intervals.
(g) the Simpson's Third Order method with 99 intervals.
(h) the Simpson's Fourth Order method with 100 intervals.
(i) Gaussian quadrature of sixth order.
(j) the cdf command in MatLab.
(k) Comment on the effect of number of intervals and order of the method.

Problem Two.
Consider the van der Waals equation of state.

$$P = \frac{RT}{\underline{V}-b} - \frac{a}{\underline{V}^2}$$

where P is pressure (Pa), T is temperature (K), $\underline{V}$ is molar volume (m^3/mol), R is the gas constant (8.314 J/mol/K = 8.314 Pa*m^3/mol/K), a is the van der Waal's attraction constant (0.2303 Pa*m^6/mol^2 for methane) and b is the van der Waal's repulsion constant (4.306×10^{-5} m^3/mol for methane).
The entropy change upon expanding is

$$\Delta S = \int_{\underline{V}_1}^{\underline{V}_2} \left(\frac{\partial P}{\partial T}\right)_{\underline{V}'} d\underline{V}'$$

where

$$\left(\frac{\partial P}{\partial T}\right)_{\underline{V}} = \frac{R}{\underline{V}-b}$$

Find the entropy change upon expanding methane from 0.05 to 0.11 m^3/mol at T = 298 K.

(a) Find analytical integral.
(b) Find the integral using Gaussian quadrature.
(c) Find the integral using the data provided in 'file.hw11p02c.txt'.
(d) Repeat part (a) at T = 398 K. Comment