Homework 2

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1 Problem 1

1.1 1(a)

We are to find the density of states of hypercubic lattice. Give

$$\rho_{d\to\infty}(\epsilon) = \lim_{d\to\infty} \int \frac{d^dk}{(2\pi)^d}\delta(\epsilon - \epsilon_k).$$

Plug in everything given by Jim, we obtain

$$\rho_{d\to\infty}(\epsilon) = \lim_{d\to\infty} \int \frac{d^dk}{(2\pi)^d}\frac{1}{2\pi}\int_{-\infty}^{\infty} d\lambda e^{-i\lambda(\epsilon+2t\sum_{i=1}^{d}\cos k_i)}. \tag{1}$$

For the first Brillouin Zone, we integrate k from $-\pi$ to π. And after rearranging equation 1, we have

$$\rho_{d\to\infty}(\epsilon) = \lim_{d\to\infty} \int_{-\pi}^{\pi} d^dk\frac{1}{(2\pi)^d}e^{-i\lambda(2t\sum\cos k_i)}\int_{-\infty}^{\infty} d\lambda e^{-i\lambda\epsilon}\frac{1}{(2\pi)}. \tag{2}$$

By looking at the first part of this integral, we notice that

$$\int_{-\pi}^{\pi} d^dk\frac{1}{(2\pi)^d}e^{-i\lambda(2t\sum\cos k_i)} = \left[\int_{-\pi}^{\pi} dk\frac{1}{2\pi}e^{-i\lambda 2t\cos k}\right]^d, \tag{3}$$

assuming $k_1 = k_2 = k_3 = ... = k_i$ (given the name of this lattice hyper**cubic**, I think this assumption is legit). Equation 3 is then the zeroth order Bessel function, which in power series takes the form

$$J_0(z) = \sum_{k=0}^{\infty}(-1)^k\frac{(\frac{1}{4}z^2)^k}{(k!)^2}. \tag{4}$$

Now substitute this into equation 3, we get

$$\left[\int_{-\pi}^{\pi} dke^{-i\lambda 2t\cos k}\right]^d = \left[\int_{-\pi}^{\pi} dke^{-i\lambda\frac{t^*}{\sqrt{d}}\cos k}\right]^d = \left[\sum_{k=0}^{\infty}(-1)^k\frac{(\frac{1}{4}(\frac{\lambda t^*}{\sqrt{d}})^2)^k}{(k!)^2}\right]^d.$$

Expand the series, we get

$$\left[1+(-1)\frac{1}{4}\frac{\lambda^2(t^*)^2}{d}+...\right]^d.$$

If we take the limit $d\to\infty$, and use the hint, we get

$$\lim_{d\to\infty}\left[\int_{-\pi}^{\pi} dke^{-i\lambda 2t\cos k}\right]^d = \lim_{d\to\infty}\left[1+(-1)\frac{1}{4}\frac{\lambda^2(t^*)^2}{d}+...\right]^d = exp(-\frac{\lambda^2(t^*)^2}{4}).$$

Substitute this into equation (2),

$$\rho_{d\to\infty}(\epsilon) = \int_{-\infty}^{\infty} d\lambda e^{-\frac{\lambda^2 (t^*)^2}{4}} e^{-i\lambda\epsilon} \frac{1}{2\pi},$$

we want to complete the square for the exponent and use Gaussian integral,

$$\rho_{d\to\infty}(\epsilon) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\lambda exp(-\frac{(t^*)^2\lambda^2}{4} - i\lambda\epsilon) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\lambda exp(-\frac{(t^*)^2}{4}(\lambda^2 + i\frac{2\epsilon}{(t^*)^2})^2 - \frac{\epsilon^2}{(t^*)^2}).$$

Use Gaussian integral formula, we obtain

$$\rho_{d\to\infty}(\epsilon) = \frac{1}{2\pi} e^{-\frac{\epsilon^2}{(t^*)^2}} \frac{2\sqrt{\pi}}{t^*} = \boxed{e^{-\frac{\epsilon^2}{(t^*)^2}} \frac{1}{t^*\sqrt{\pi}}}.$$

1.2 1(b)

Here we let $t^* = 1$, making it our energy unit.
For the 1-D model, the density of states goes to infinity at both edges. The 2-D density of states are discontinuous (although it seems continuous in the graph) at $E = 0$. The 3-D and infinite-D models both have DOS going to zero at band edges. It if fair to say that as $d \to \infty$, the density of states can be treated like the one for the 3-D case.

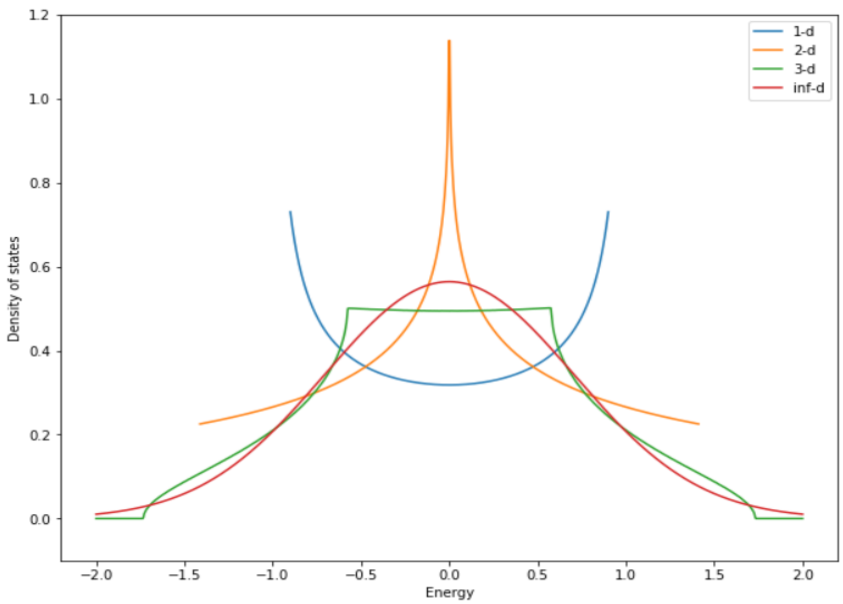


Figure 1: Density of states for 1-d, 2-d, 3-d, and infinite-dimension, using $t^* = 2\sqrt{d}t$ as the energy unit.

1.3 1(c)

From Economou, the local Green's function for the Bethe lattice is

$$G(l, l; z) = \frac{2K}{(K-1)z + (K+1)\sqrt{z^2 - 4KV^2}}. \tag{5}$$

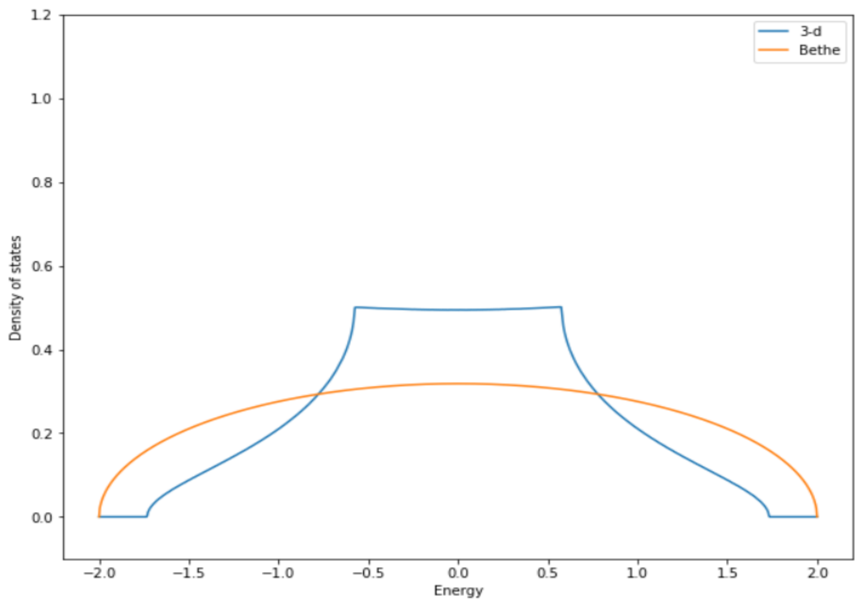
Then the density of states is given as

$$-\frac{1}{\pi}\,\text{Im}\{G(l,l;z)\} = \frac{1}{\pi}\frac{2K\sqrt{4KV^2-\epsilon^2}}{(K-1)^2\epsilon^2 + Z^2(4KV^2-\epsilon^2)}. \tag{6}$$

If we send Z ($K = Z - 1$) to ∞, and let $V = \frac{1}{\sqrt{Z}}$, we get

$$DOS_{Bethe}(\epsilon) = \frac{\sqrt{4-\epsilon^2}}{2\pi}. \tag{7}$$

Similar to the 3-D density of states, Bethe lattice DOS goes to zero near the band edges. Maybe we can approximate the Bethe lattice with $Z \to \infty$ as 3-D tight-binding model?



2 Problem 2

Here I will use

$$U = 2\int d\epsilon \rho(\epsilon)\epsilon f(\epsilon)$$

to calculate the internal energy for each dimension, where $\rho(\epsilon)$ is the density of states, and $f(\epsilon)$ is the Fermi-Dirac distribution

$$f(\epsilon) = \frac{1}{1+e^{(\epsilon-\mu)/T}}.$$

To get U, we need the chemical potential μ to calculate the distribution, which is obtained from

$$n = 2\int d\epsilon \rho(\epsilon) f(\epsilon),$$

with given values of n. The strategy is simply using a built-in root finder found in Scipy library. The entropy is calculated using

$$S = -2\int d\epsilon \rho(\epsilon)(f(\epsilon)ln(f(\epsilon)) + (1-f(\epsilon))ln(f(\epsilon))).$$

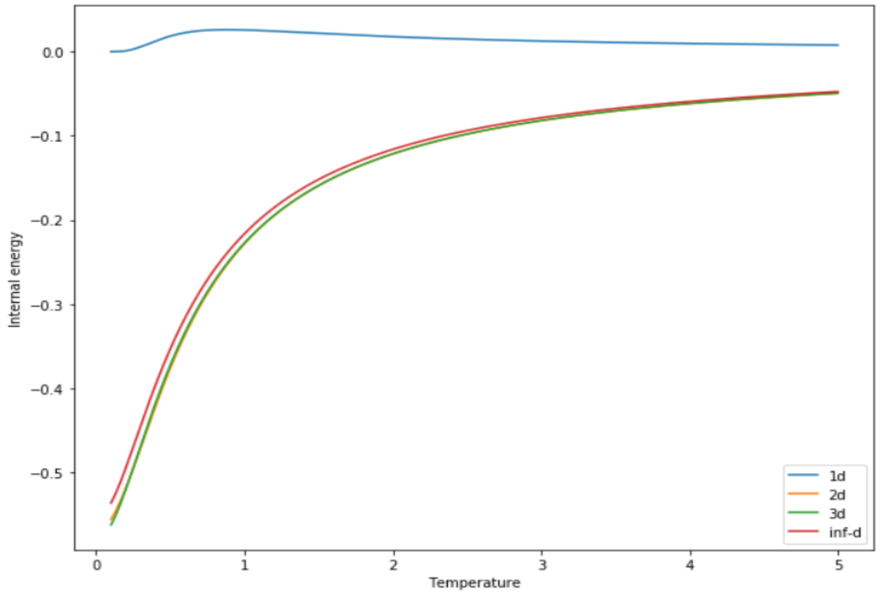
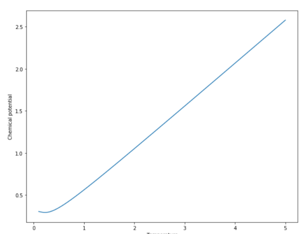
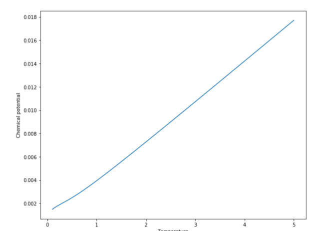


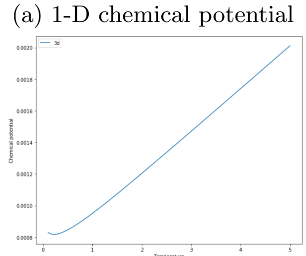
Figure 2: Internal energy with $n = 1$. Every dimension except for the 1-D case seems to have the same internal energy. I don't think it's done right. Here I'll attach a set of graphs of chemical potentials.



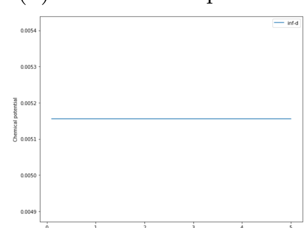
(a) 1-D chemical potential



(b) 2-D chemical potential



(c) 3-D chemical potential



(d) Infinite-D chemical potential

The free energy is found by

$$F = U - TS.$$

Then we switch to $n = 1/2$.

Here we can see for the $n = 0.5$ case, there's no convergence on the quantities that show strong convergence for the $n = 1$ case, meaning there's a phase transition at $n \geq 0.5$.

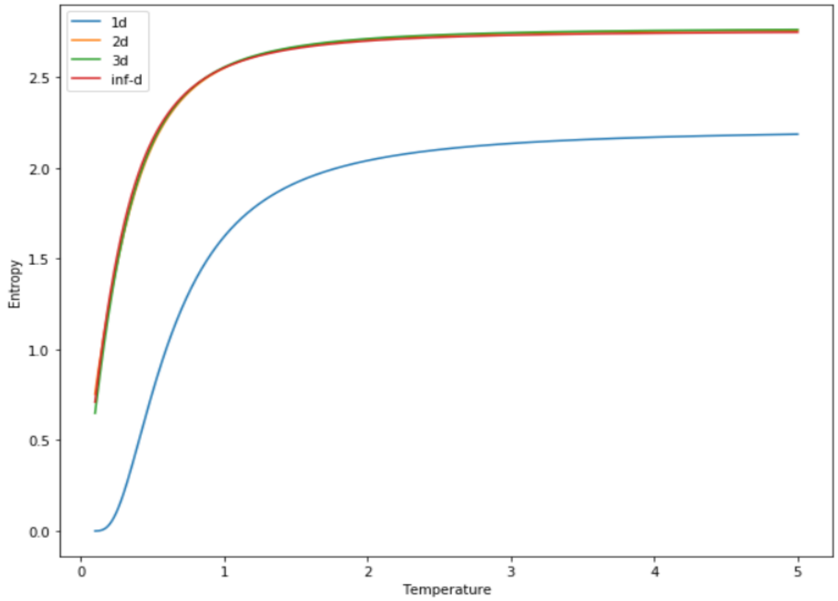


Figure 4: Entropy vs. temperature with $n = 1$, again, everything except the 1-D model seems to converge, intuitively not quite right*.

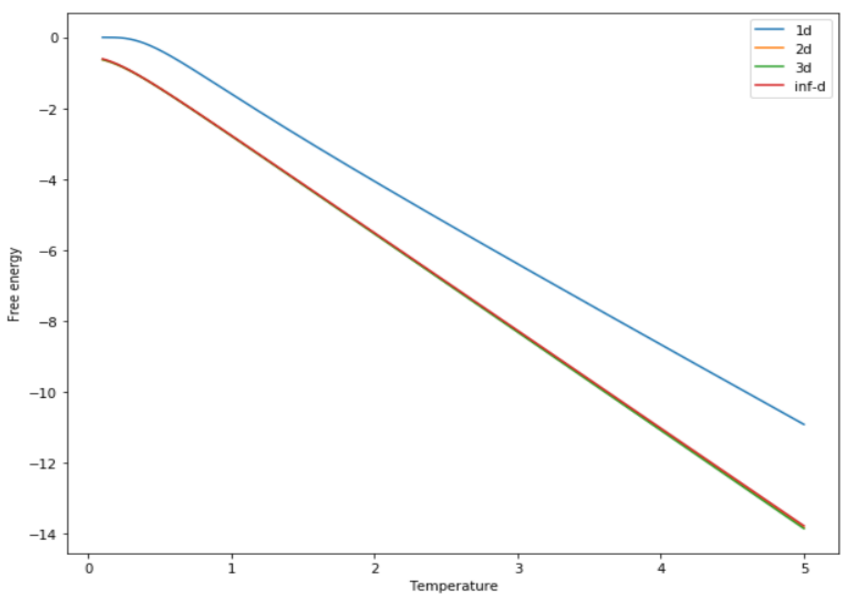


Figure 5: Free energy vs. temperature, with $n = 1$.

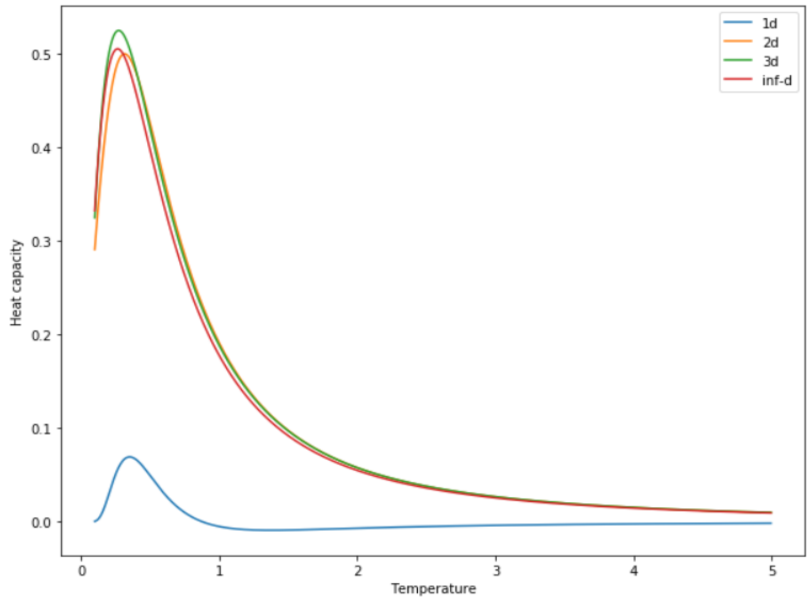


Figure 6: Heat capacity vs. temperature, with $n = 1$ calculated numerically using the symmetric definition of derivatives.

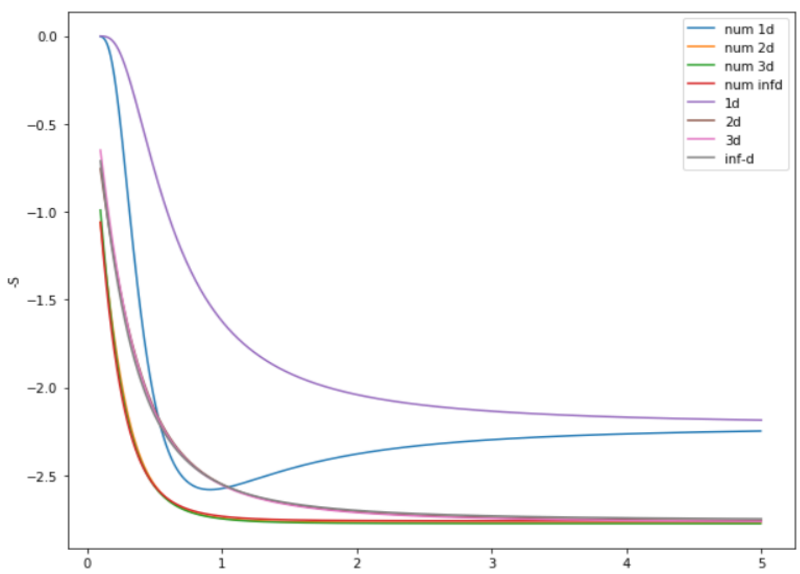


Figure 7: -S vs. temperature, with $n = 1$. For the 1-D case, the numerical result is different from the derivative significantly. For the other cases, numerical results agree with the derivatives.

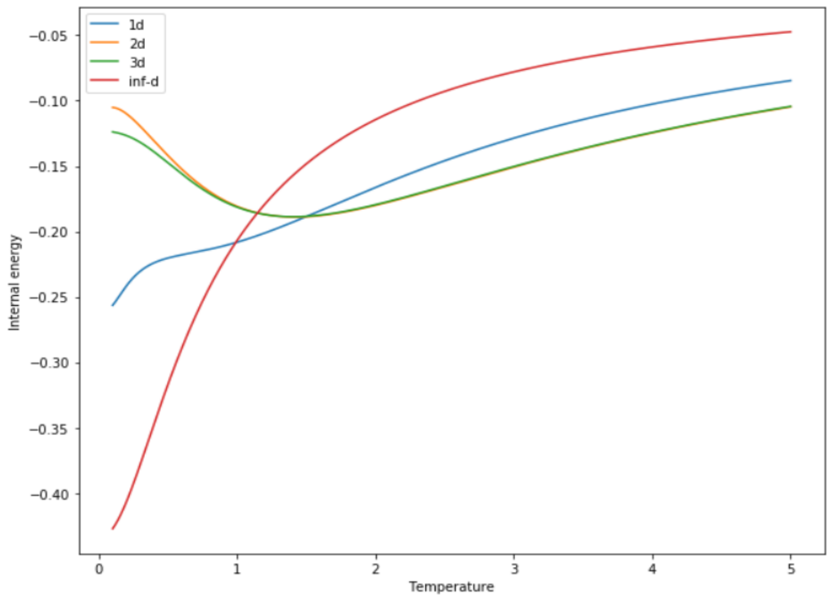


Figure 8: Internal energy vs. temperature, with $n = 0.5$.

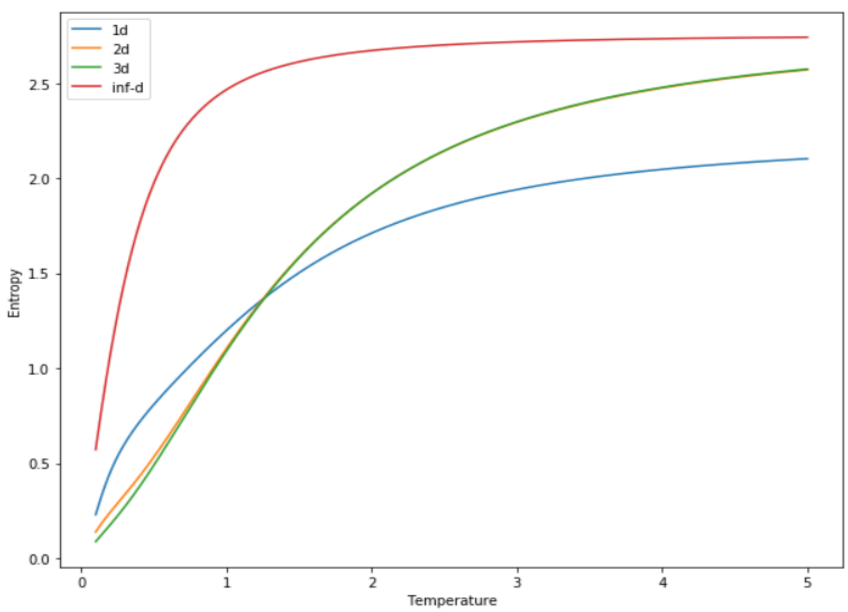


Figure 9: Entropy, with $n = 0.5$.

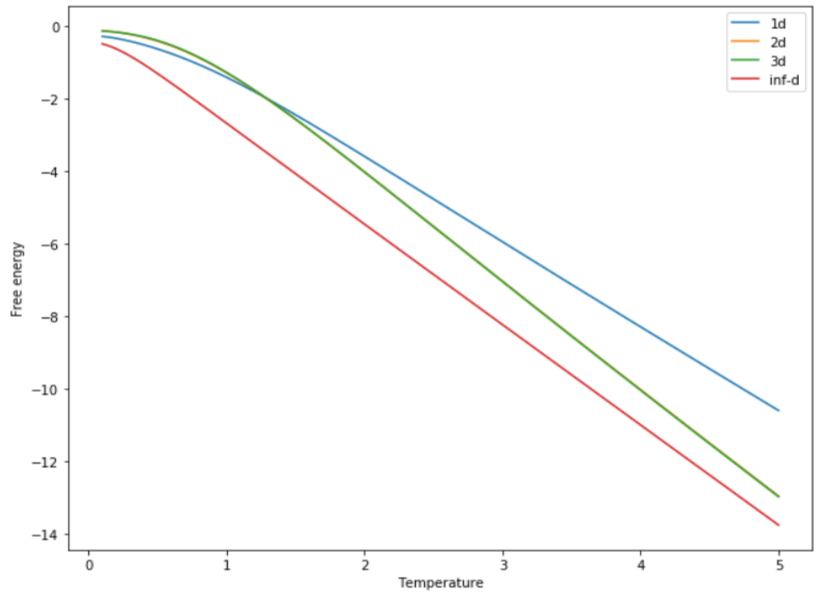


Figure 10: Free energy, with $n = 0.5$.

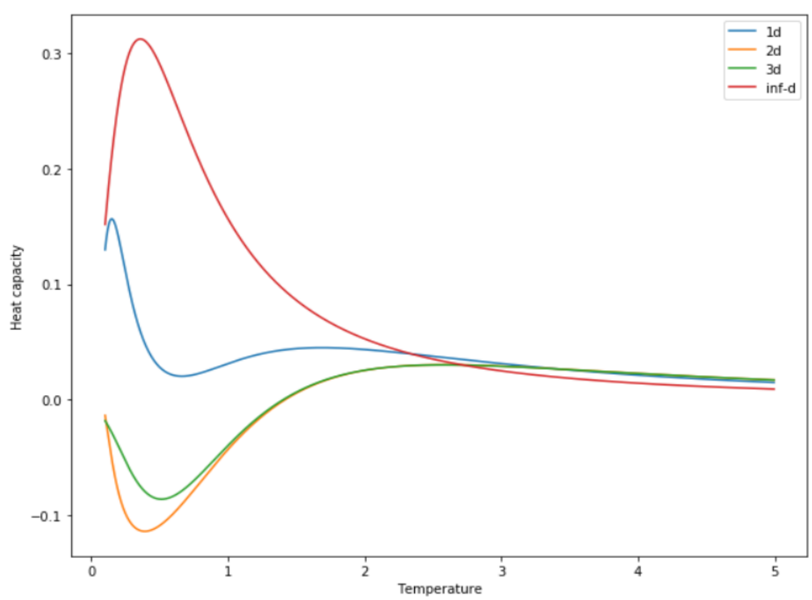


Figure 11: Heat capacity, with $n = 0.5$.

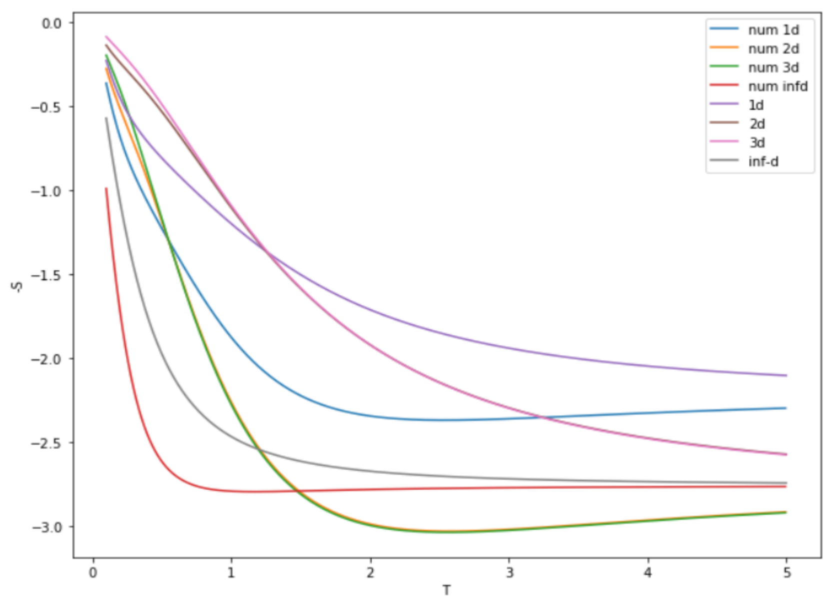


Figure 12: -S vs. temperature, using integration and derivatives.