Computational Method 2 Spring 2025

HW2

Q1 Adaptive Simpson's Rule for Numerical Integration

- Derive **Simpson's Rule** for numerical integration:

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right].$$

  Hint: Follow class notes and use a quadratic interpolating polynomial.

- Show that the local error of a single Simpson's step is

$$E_S = -\frac{(b-a)^5}{90} f^{(4)}(\xi), \quad \text{for some } \xi \in (a,b).$$

- Write a program to integrate a given function $f(x)$ over an interval $[a,b]$ using **Adaptive Simpson's Rule**. Your implementation should:
  - **Recursively** subdivide the interval if the estimated error is above a given tolerance.
  - Stop subdividing when the error estimate is below the given tolerance.
  - Return the final numerical result and the number of function evaluations used.

- Use your implementation to compute the following integral:

  The thermal pressure of a fermion gas (per flavor, per spin) is given by

$$P_F = \frac{1}{8\pi^3}\int_0^\infty dp\,4\pi p^2\,\frac{p^2}{3E(p)}\,\frac{1}{e^{\beta E(p)}+1}$$

  where $\beta = \frac{1}{T}$ and $E(p) = \sqrt{p^2+m^2}$. (All in units of GeVs) Compute this integral numerically using **Adaptive Simpson's Rule** for different temperatures (T).
  Verify that at large T

$$P_F \approx \frac{7}{8}\frac{\pi^2}{90}T^4.$$

Q2 Low and High Temperature expansions.

- Fill in the steps in deriving the exact solution of the 1D Ising Model based on Transfer Matrix method. Obtain the analytic expressions of the partition function and average spin.

- Compare the results to the corresponding low and high temperature expansions of the partition function.
- Derive the low and high temperature expansions of the energy per site for the d-dimensional Ising Model at zero external field.

Q3 2D Ising Model.

- Write down the partition function in the low and high temperature expansions (at least 2 correction terms in each case).
- Compare the correction factors to the corresponding leading term. Show that the two series are the same if we map

  $$e^{-2K} \leftrightarrow \tanh(K).$$

  Plot the two functions versus K.
- Obtain an analytic expression of the critical coupling K_c at the point of intersection. (K is just the inverse temperature for $J = 1$)
- The exact solution, due to Onsager, for the partition function reads (see textbook by Pathria or Kerson Huang)

  $$\begin{aligned} \ln Z_{\text{persite}} &= \ln\left(\sqrt{2}\cosh 2K\right) + \frac{1}{\pi}\int_0^{\pi/2} d\phi \ln\left(1 + \sqrt{1 - \kappa^2 \sin^2\phi}\right) \\ \kappa &= \frac{2\sinh 2K}{\cosh^2 2K}. \end{aligned}$$

  Derive and Plot the exact solution for energy per site versus temperature. Compare with the low and high temperature expansions.