Free energy estimate by thermodynamic integration.

Write a MD or Lajevin code sampling the canonical probability distribution at a temperature T=1 of a three-dimensional potential of the form

$$V\left(x,y\right)=-5\log\left(3\exp\left(-2x^{2}-\frac{1}{4}y^{2}-z^{2}\right)+2\exp\left(-\left(x-\frac{3}{2}\right)^{2}-\left(y-\frac{5}{2}\right)^{2}-z^{2}\right)\right)$$

1. Compute the free energy $F\left(s\right)$ as a function of the collective variable $s=x^{2}+y^{2}$ by thermodynamic integration.
2. Estimate the error of the derivative of the free energy for each value of the CV, and estimate the error on the free energy difference $F(10)-F(0)$ by error propagation.
3. Estimate the error on the same free energy difference by performing a thermodynamic cycle. Comment