# MCMD w3 – Protein Fibril Formation

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April 26, 2019

We compare the obtained estimates of $\ln g(E)$ for systems A (1D) and B (2D), see Fig 1, for the last five iterations in $f$ for each to evaluate the convergence. From the figure we find that the estimates have converged in both systems.

## 1 Heat capacity

Using the converged estimates for both systems we estimate the respective heat capacities. Note that due to considerations of unphysical cyclical aggregates we omit temperatures where the probabilities $P_T(E = -699)$ or $P_T(E = -698)$ are above the threshold $10^{-4}$. The heat capacities are provided in Fig. 2. The heat capacity is maximised at the points $T_A = 0.650$ for system A and $T_B = 0.657$ for B.

## 2 Probability distribution

Finally, we construct the probability distribution functions (PDFs) for the systems at the temperatures that maximises the respective heat capacities. The data is smoothed in bins of width 4, see Fig 3. For a system with an abrupt transition between the disordered solution and the mixed state one expects a bimodal energy distribution. According to the obtained PDFs system A is unimodal while B is bimodal.
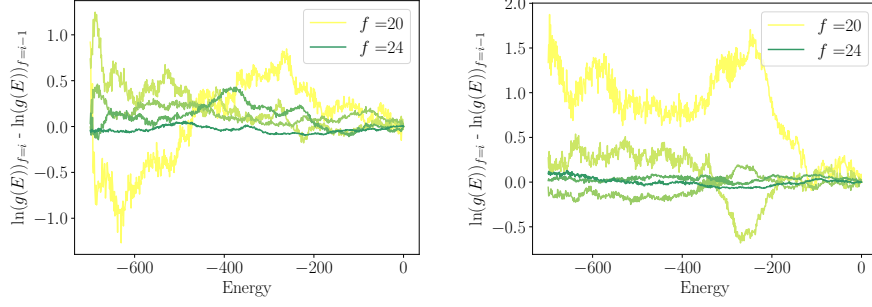
Figure 1: Difference between iterations for last five $f$-values in the Wang-Landau estimation of $\ln g(E)$ for systems A (left) and B (right), respectively. The colour changes from yellow to green as we convergence settles.
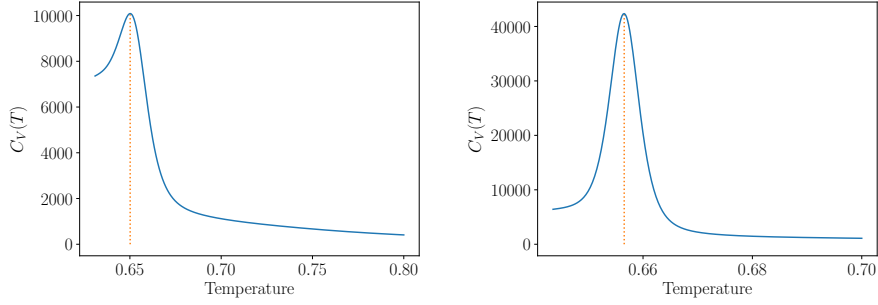


Figure 2: Heat capacity for temperatures with physical solutions for system A (left) and B (right)
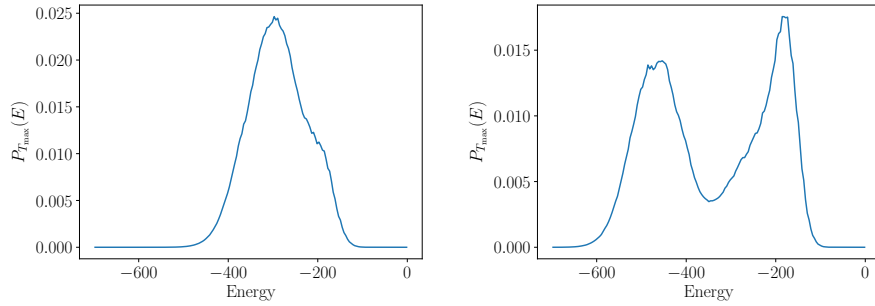


Figure 3: Probability distributions at maximum temperatures for system A (left) and B (right).