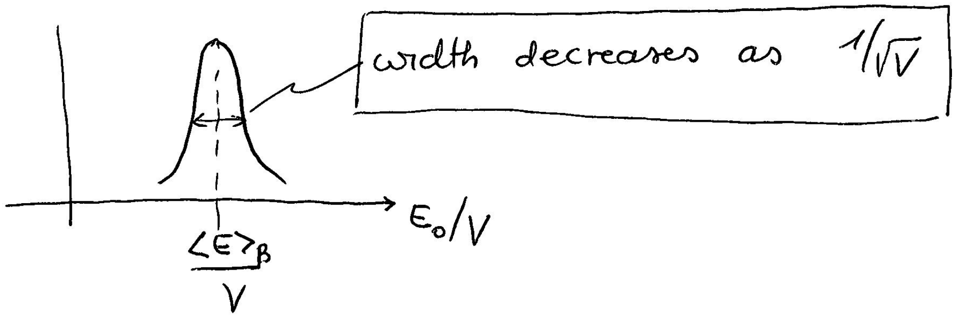
OPTIMIZATION OF THE UMBRELLA DISTRIBUTION

For a canonical distribution

$$\langle \delta_{E,E_0} \rangle_\beta = h(E_0,\beta) = \frac{1}{Z_\beta} \int dE \, \rho(E) e^{-\beta E} \delta_{E,E_0}$$

$$= \frac{1}{Z_\beta} \rho(E_0) e^{-\beta E_0}$$

Plot of $h(E_0,\beta)$



NOTE: The coefficients a_i in these notes correspond to the coefficients alpha_i of the notes of the previous lesson

For the umbrella distribution

$$h_\pi(E_0) = \frac{1}{Z_\pi} \sum_x \left(\sum_i a_i e^{-\beta_i H(x)} \right) \delta_{E,E_0}$$

$$= \frac{1}{Z_\pi} \sum_E \rho(E) \left(\sum_i a_i e^{-\beta_i E} \right) \delta_{E,E_0}$$

$$= \frac{1}{Z_\pi} \rho(E_0) \sum_i a_i e^{-\beta_i E_0}$$

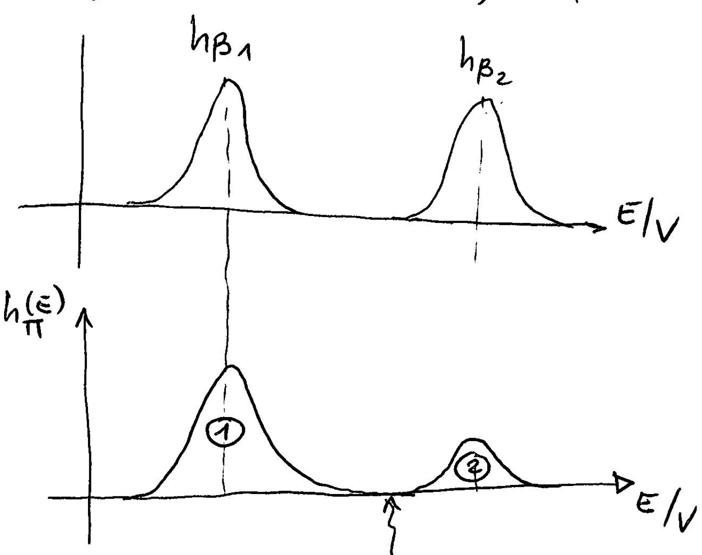
$$= \frac{1}{Z_\pi} \sum_i a_i Z_{\beta_i} \left(\frac{1}{Z_{\beta_i}} \rho(E_0) e^{-\beta_i E_0} \right)$$

$$= \frac{1}{Z_\pi} \sum_i a_i Z_{\beta_i} h_{\beta_i}(E_0)$$

$$h_\pi(E_0) = \sum_i \frac{a_i Z_{\beta_i}}{Z_\pi} h_{\beta_i}(E_0) = \sum_i c_i h_{\beta_i}(E_0) \qquad \left(\sum c_i = 1\right)$$

$h_\pi(E_0)$ is a linear combination of the h_{β_i}

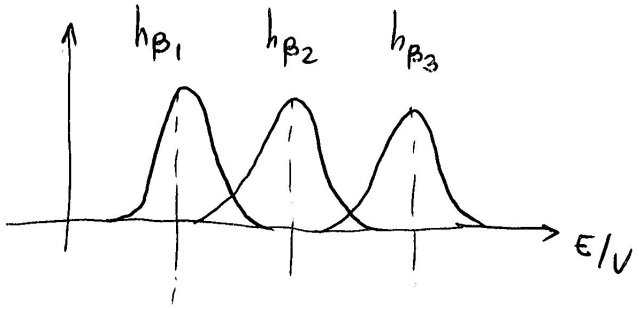
1. The algorithm works only if distributions overlap



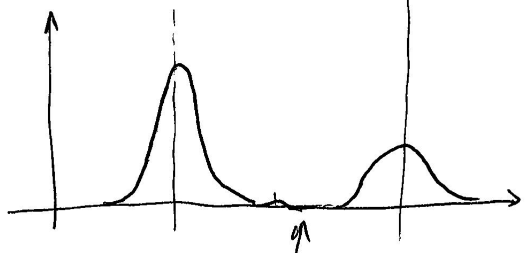
probability to be here ≈ 0
As E changes slowly in the MC simulations, a simulation that starts in 1 never visits 2 and viceversa

Distributions <u>MUST</u> overlap

2



Now assume $c_1 = 0.7$ $c_2 = 10^{-4}$ $c_3 = 0.3 - 10^{-4}$



the probability to go through configurations that are typical at inverse temperature β_2 is tiny.

Requirement: the optimal behavior is obtained if all c_i are (approximately equal)

$$\frac{a_i \, Z_{\beta_i}}{Z_\pi} \approx \frac{a_j \, Z_{\beta_j}}{Z_\pi} \Rightarrow \frac{a_i}{a_j} = \frac{Z_{\beta_j}}{Z_{\beta_i}}$$

IMPLEMENTATION

a) Given β_{min}, β_{max}, the β-interval we wish to cover define

$$\beta_1 = \beta_{min}\,,\ \beta_2 \dots \quad \beta_N = \beta_{max}$$

so that the energy distributions overlap

NOTE: the number of β_i's should increase as the volume increases as the distribution of E/V shrinks as $1/\sqrt{V}$

b) Perform short runs at $\beta_1 \dots \beta_N$ to compute

$$\frac{Z_{\beta_{i+1}}}{Z_{\beta_i}} \quad \text{so that} \quad a_{i+1} = \frac{Z_{\beta_i}}{Z_{\beta_{i+1}}}\, a_i$$

$\boxed{\text{Fix } a_1 = 1} \longrightarrow$ compute all a_i

c) Start the simulation with the umbrella distribution

The UMBRELLA DISTRIBUTION CAN BE OPTIMIZED DURING THE RUN

$$\frac{Z_{\beta_i}}{Z_{\beta_j}} = \frac{\left\langle \dfrac{e^{-\beta_i H}}{\sum_K a_K e^{-\beta_K H}} \right\rangle_\pi}{\left\langle \dfrac{e^{-\beta_j H}}{\sum_K a_K e^{-\beta_K H}} \right\rangle_\pi}$$