

## Histogram Monte Carlo (Ferrenberg & Swendsen)

$$Z = \int dE \Omega(E) e^{-\beta E}$$

$$U = \langle E \rangle = \int dE \Omega(E) \cdot E \cdot e^{-\beta E} / Z$$

$\left. \begin{array}{l} \Omega(E) = \text{density of states} \\ P(E) = \Omega(E) e^{-\beta E} / Z \end{array} \right\}$

$\uparrow$  Sums if  $E$  discrete

Monte Carlo histogram  $H(E) \sim P(E)$  unknown constant of proportionality

$$H(E) = C \cdot P(E) \Rightarrow C = \int dE H(E)$$

$$U = \int dE \cdot E \cdot H(E) / \int dE H(E)$$

$\uparrow$  Standard M.C.  $C$  cancels out

Invert  $P(E) = \frac{1}{Z} \Omega(E) e^{-\beta E}$

$$\Rightarrow \Omega(E) = Z P(E) e^{+\beta E} = C' H(E) e^{\beta E} \quad C' = C Z$$

Given simulation at  $\beta_0 = \frac{1}{kT_0} \Rightarrow \frac{1}{C'} \Omega(E)$  over sampled  $E$  range

$$\begin{aligned} \text{Then } U(T_1) &= \int dE \left( \frac{1}{C'} \Omega(E) \right) \cdot E \cdot e^{-\beta_1 E} / \int dE \left( \frac{1}{C'} \Omega(E) \right) e^{-\beta_1 E} \\ &= \int dE H(E) \cdot E \cdot e^{-(\beta_1 - \beta_0) E} / \int dE H(E) e^{-(\beta_1 - \beta_0) E} \end{aligned}$$

Can also get  $C(T_1)$  from  $\langle E^2 \rangle - \langle E \rangle^2$

2D Histograms  $H(E, M) \leftarrow$  MC at  $T_0$  and  $h_0$

$$M(T_1, h_1) = \int dE dM \cdot M \cdot H(E, M) e^{-[\Delta\beta E - \Delta(\beta h) M]} / \int dE dM H(E, M) e^{-\dots}$$

$\uparrow$  can get  $M(h_1)$  from MC simulation at  $h_0 = 0!$