Multicanonical Monte Carlo Simulations of the Abelian Higgs Model

Master Thesis (with Wolfhard Janke)

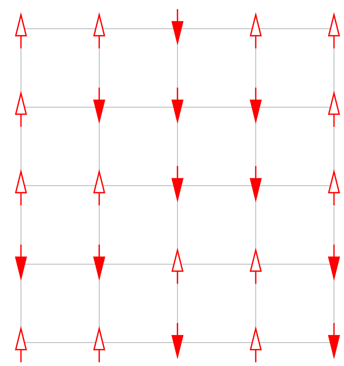
Institute of Theoretical Physics
Universität Leipzig, Germany

Outline

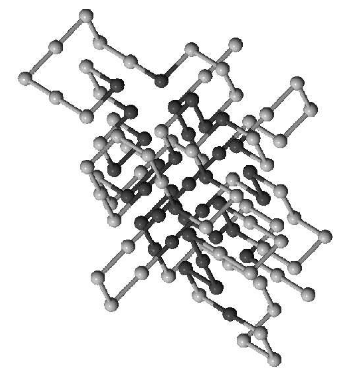
- Statistical Physics
- Phase Transition
- Markov Chain Monte Carlo
- Metropolis algorithm
- Multicanonical Metropolis
- (Application to Abelian Higgs Model)
- Summary

Framework of Statistical Physics

- Consider a many-particle physical system. A specific state of the system is a configuration c.



configuration in Ising model



configuration of an HP polymer

- Assign probability distribution $p(c)$ over space of configurations c.

$$p(c) = \frac{1}{Z} \exp\left(-\beta E(c)\right),$$

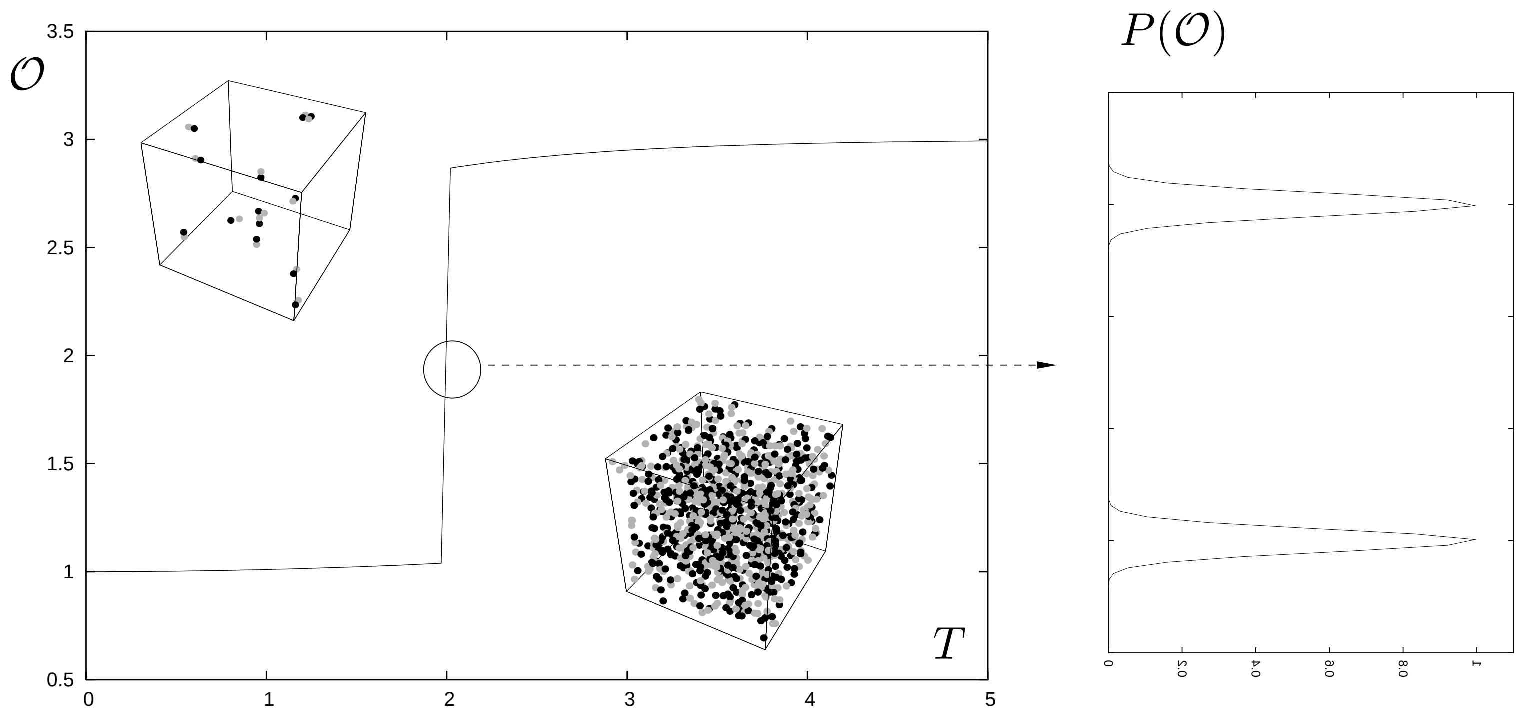
where E is the energy of the configuration and β inverse temperature

- Expectation values of observables $\mathcal{O}$:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_c \mathcal{O}(c) p(c)$$

- since configuration space very large, cannot perform calculation of expectation values exactly.

(First Order) Phase Transition



- system behaviour changes fundamentally at some temperature T
- actual point of interest in statistical physics
- first order transition $\Leftrightarrow$ finite jump
- metastability at transition point
- double peak in distribution $P(\mathcal{O})$

Markov Chain Monte Carlo

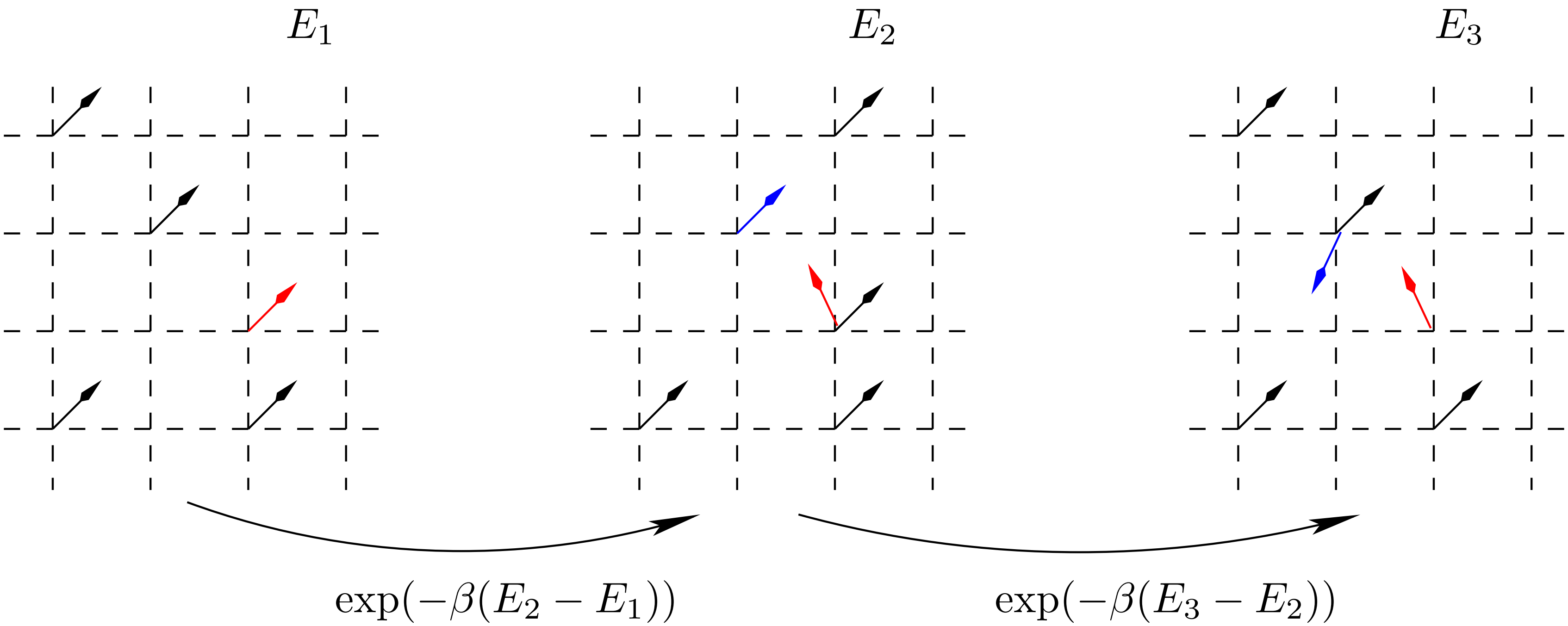
- use **stochastic** methods to generate configurations c_i from a probability distribution $\pi(c)$. Calculate an estimator for $\langle \mathcal{O} \rangle$ with

$$\bar{\mathcal{O}}_{\mathrm{E}} = \frac{\sum_i^N \pi_i^{-1} \mathcal{O}_i p_i}{\sum_i^N \pi_i^{-1}} \qquad \lim_{N\to\infty} \bar{\mathcal{O}}_{\mathrm{E}} = \langle \mathcal{O} \rangle$$

- Monte Carlo is one method specifically designed to draw huge number of samples.
  - trivial sampling
  - importance sampling
    - canonical sampling: choose $\pi = p$
    - multicanonical sampling: choose more general π
- importance sampling uses a 1st order Markov process $W(c_{n+1}|c_n)$ which drives system to equilibrium distribution $p(c)$.

$$W(c_{n+1}|c_n)p(c_n) = W(c_n|c_{n+1})p(c_{n+1})$$

Example: The Metropolis Algorithm



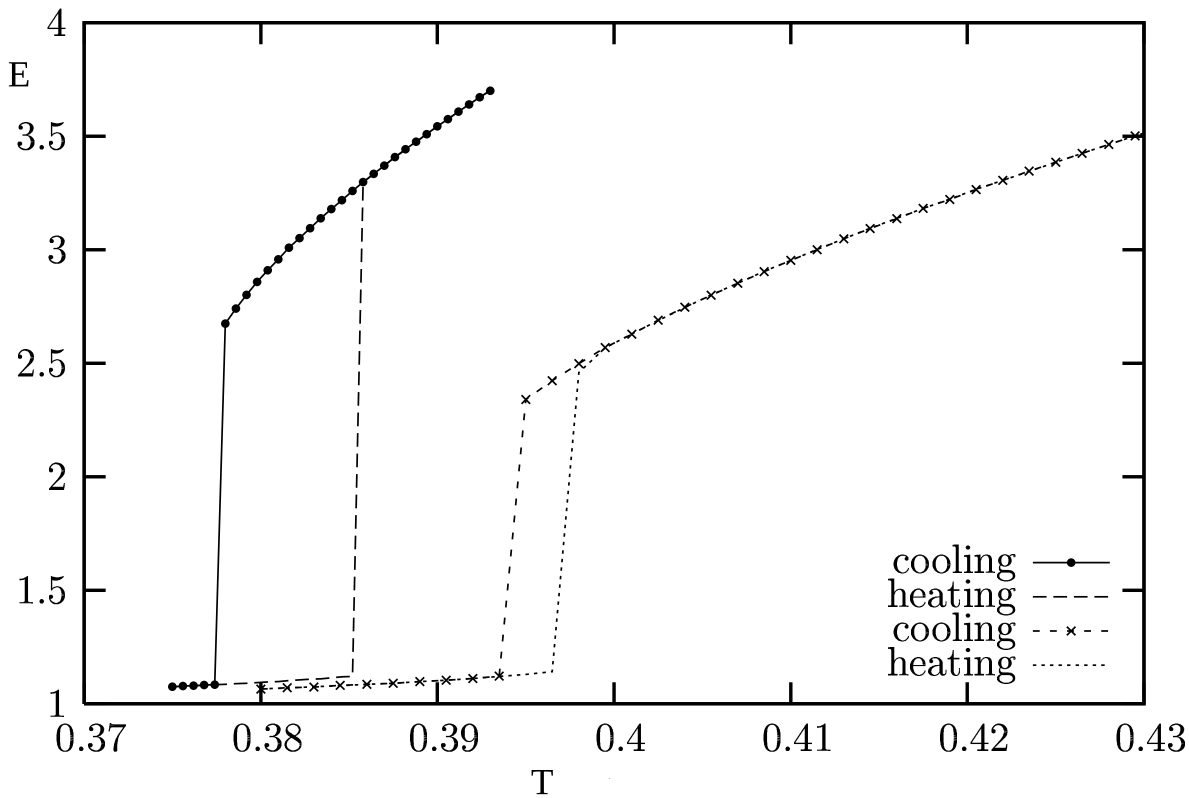
- standard example of canonical sampling
- propose move
- accept it with probability

$$W(c_{n+1}|c_n) = \min\left[1, \frac{p(c_n)}{p(c_{n+1})}\right] = \min[1, \exp(-\beta\Delta E)]$$

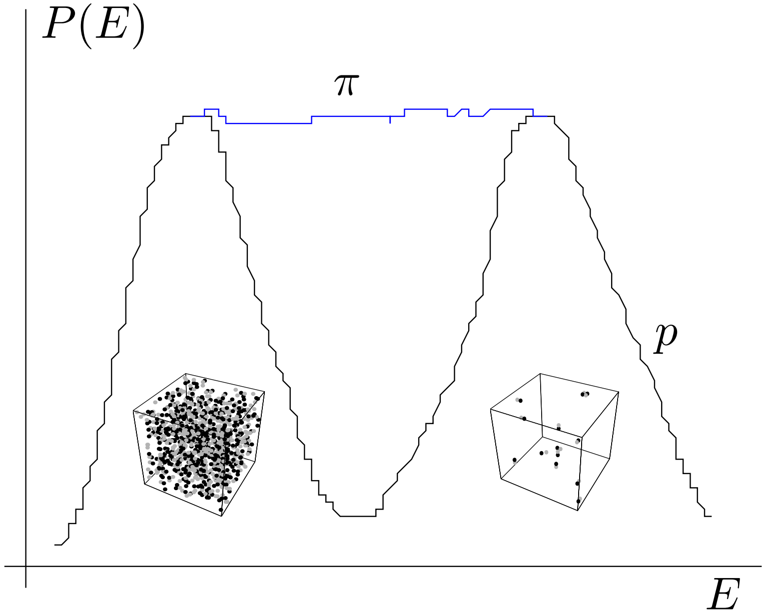
- local algorithm, need to know relative energy difference only

Metropolis at First Order Transitions

- observe typical hysteresis effects
- simple Metropolis algorithm cannot tell what the right phase is
- reason: stochastic process needs to long to sample the whole phase space (**supercritical slowing down**)



The Multicanonical Metropolis Algorithm



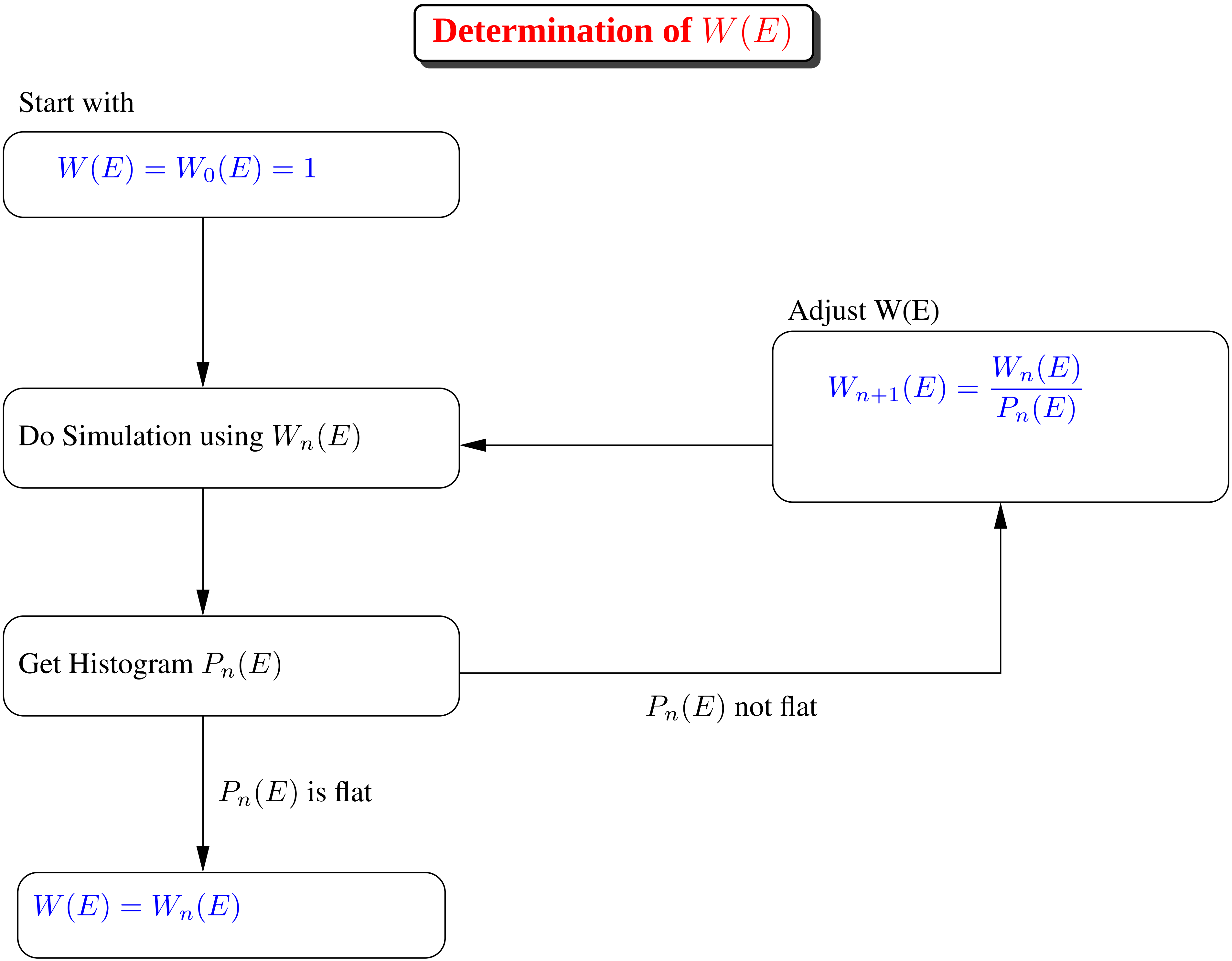
1. at first-order transitions stochastic process may be trapped in one region (probability barrier)

2. idea: can sample from a more general probability distribution $\pi(c)$

3. choose $\pi(c)$ in a way to enhance random walks through the whole configuration space (**flat histogram**)

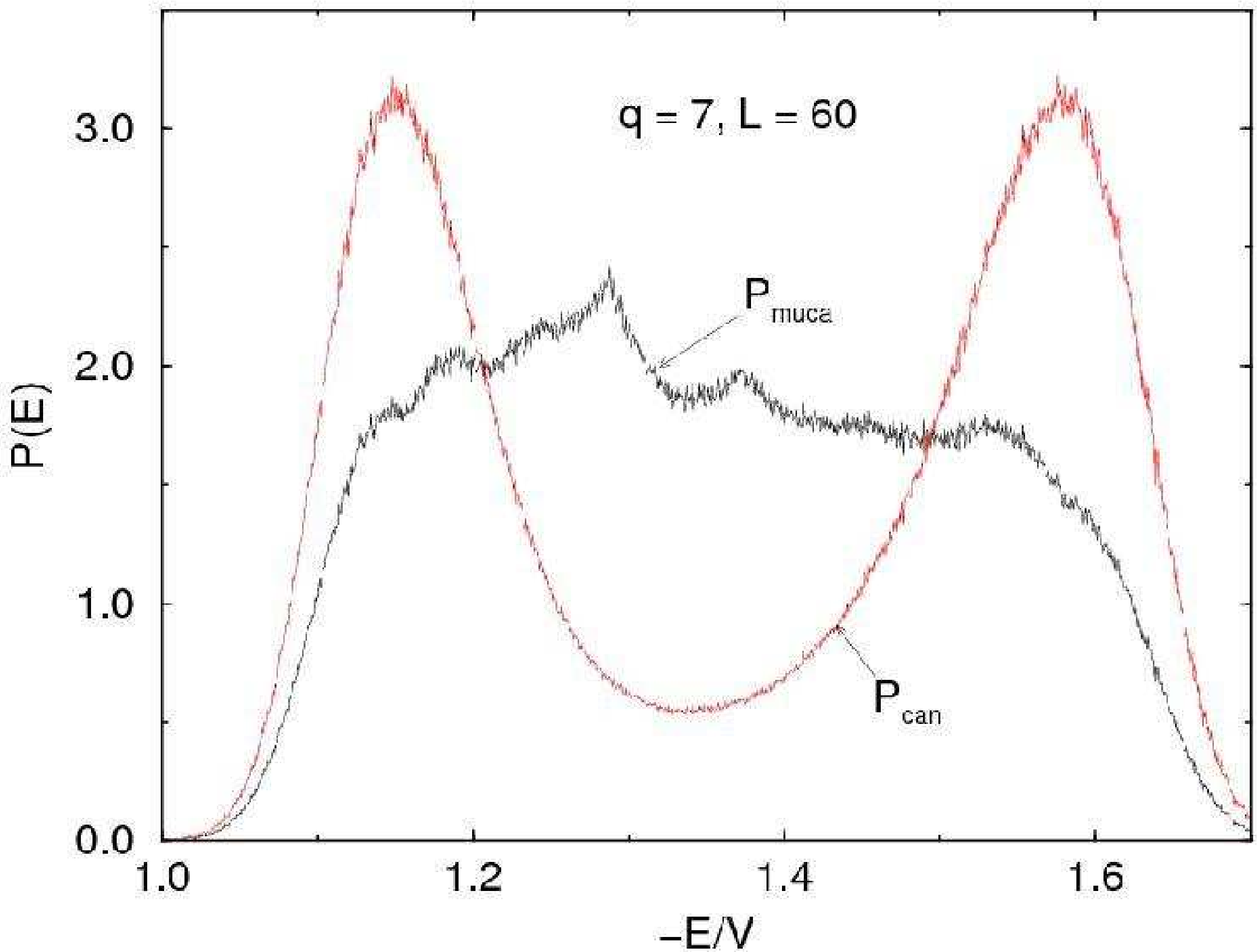
$$\pi = p \times W(E) = \exp\left(-\beta E\right) \times W(E)$$

4. need to determine $W(E)$ prior to simulation
   - self consistent approach
   - usual hardes part of simulation


Determination of $W(E)$
Start with
$W(E) = W_0(E) = 1$
Adjust W(E)
$W_{n+1}(E) = \frac{W_n(E)}{P_n(E)}$
Do Simulation using $W_n(E)$
Get Histogram $P_n(E)$
$P_n(E)$ not flat
$P_n(E)$ is flat
$W(E) = W_n(E)$

A Small Example

Example for the Potts model $q = 7$.



- here $W(E)$ has been determined separately
- $P_{\text{muca}}(E)$ measured simulation
- physical result $P_{\text{can}}(E) = P_{\text{muca}}(E)/W(E)$

Summary

- introduced idea of Monte Carlo
- Metropolis algorithm (sample from Boltzmann distribution p)
- Multicanonical algorithm (sample from $p * W(E)$)
- Multicanonical algorithm eliminates supercritical slowing down. and allows to study strong first-order transitions
- In my thesis I have applied this to the Abelian Higgs model