Monte Carlo methods in Statistical Physics

Next three lectures

1. Monte Carlo in Statistical Physics
2. Monte Carlo for optimization and simulation of evolution
3. Dynamic Monte Carlo for simulations of (bio)chemical reactions

Outline

- Ising-Lenz model of ferromagnetism
- Equilibrium, Boltzman distribution
- Computing Average
  - Simple sampling
  - Importance sampling
- Detailed balance
- Metropolis Monte Carlo algorithm

Magnetism

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See http://cwx.prenhall.com/petrucci/medialib/media_portfolio/text_images/FG24_03.JPG

Ferromagnetism

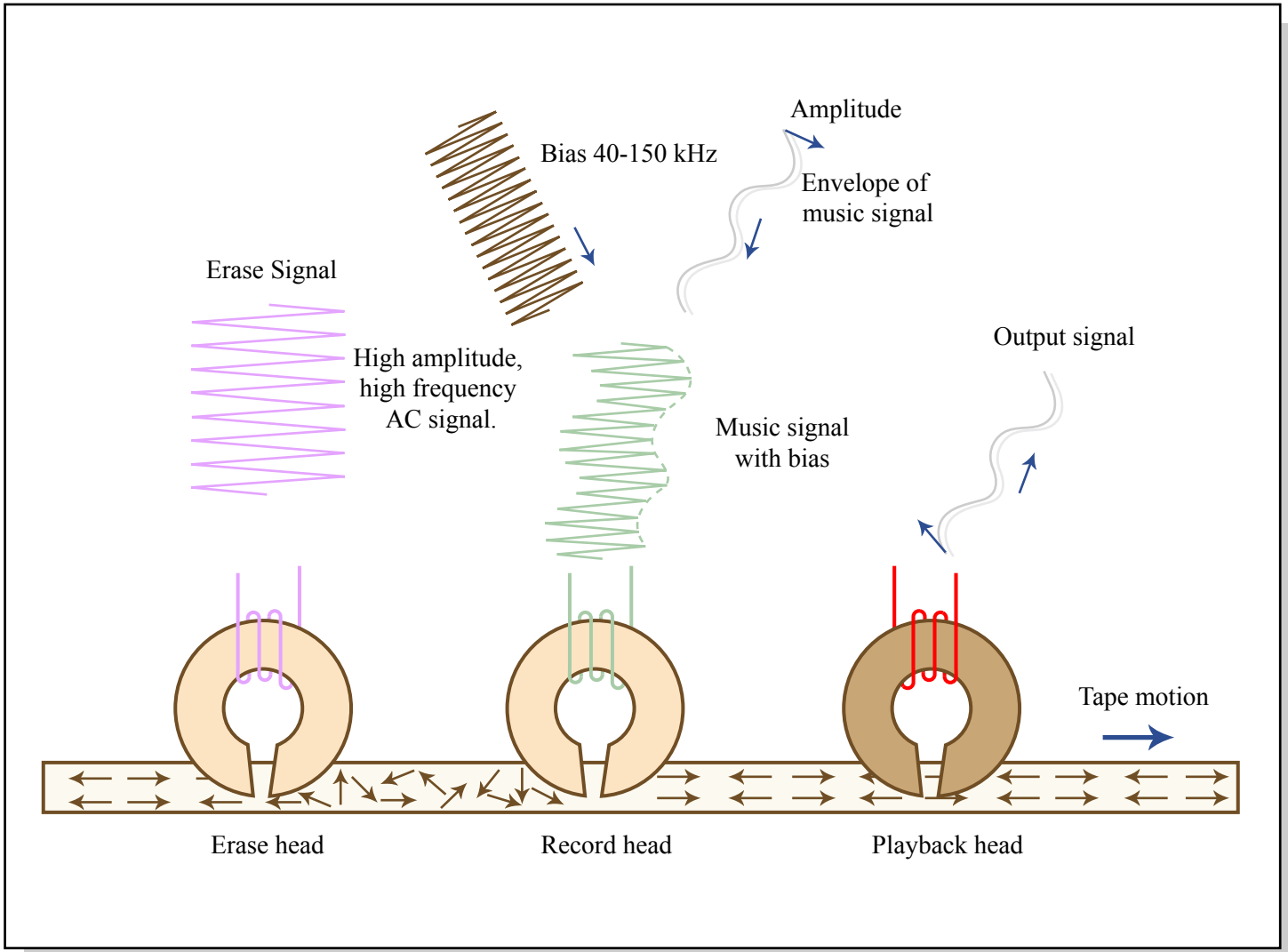

Figure by MIT OCW.

Ising-Lenz model

Spin

$$s_i = \begin{cases} +1 \\ -1 \end{cases}$$

Energy

$$E(s) = -J \sum_{(i,j)} s_i \cdot s_j - H \sum_i s_i$$

Magnetization

$$M(s) = \sum_i s_i$$

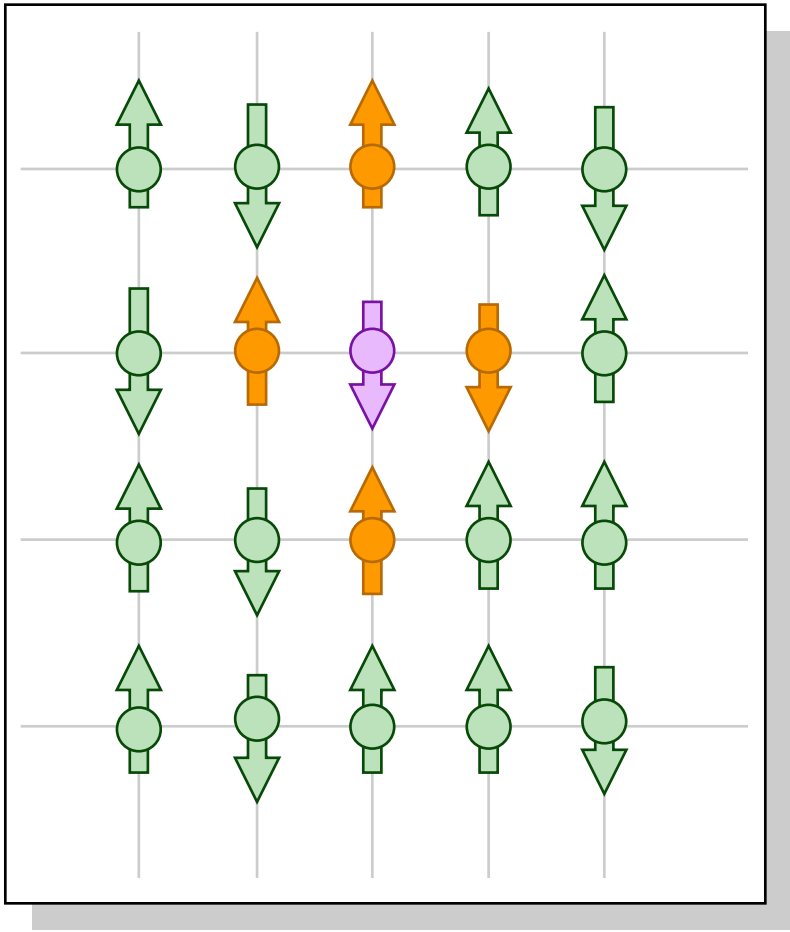

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Image of Wilhelm Lenz.

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See Fig. 7 in KOBE, S. "Ernst Ising 1900-1998." *Braz J Phys* 30 (2000): 649-654.
<http://www.scielo.br/scielo.php?script=sci_arttext&pid=S0103-97332000000400003&lng=en&nrm=iso>

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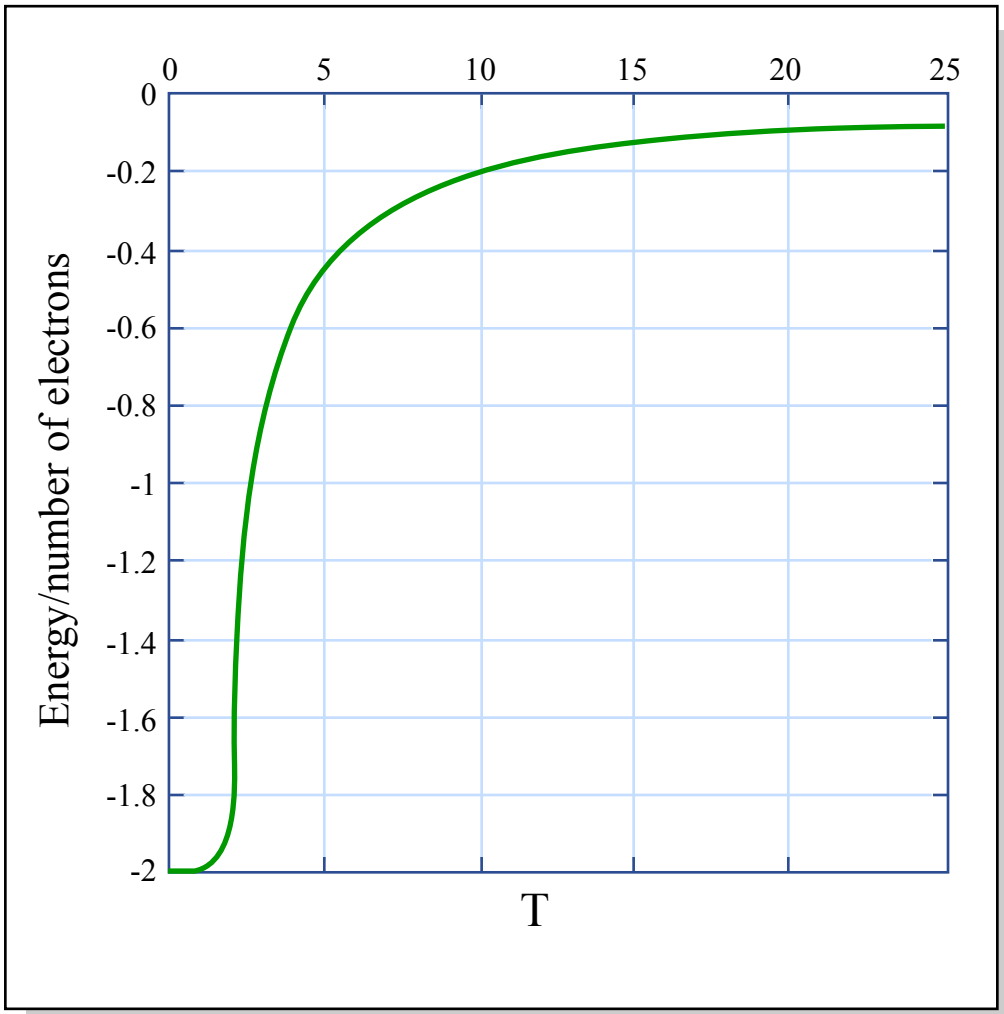
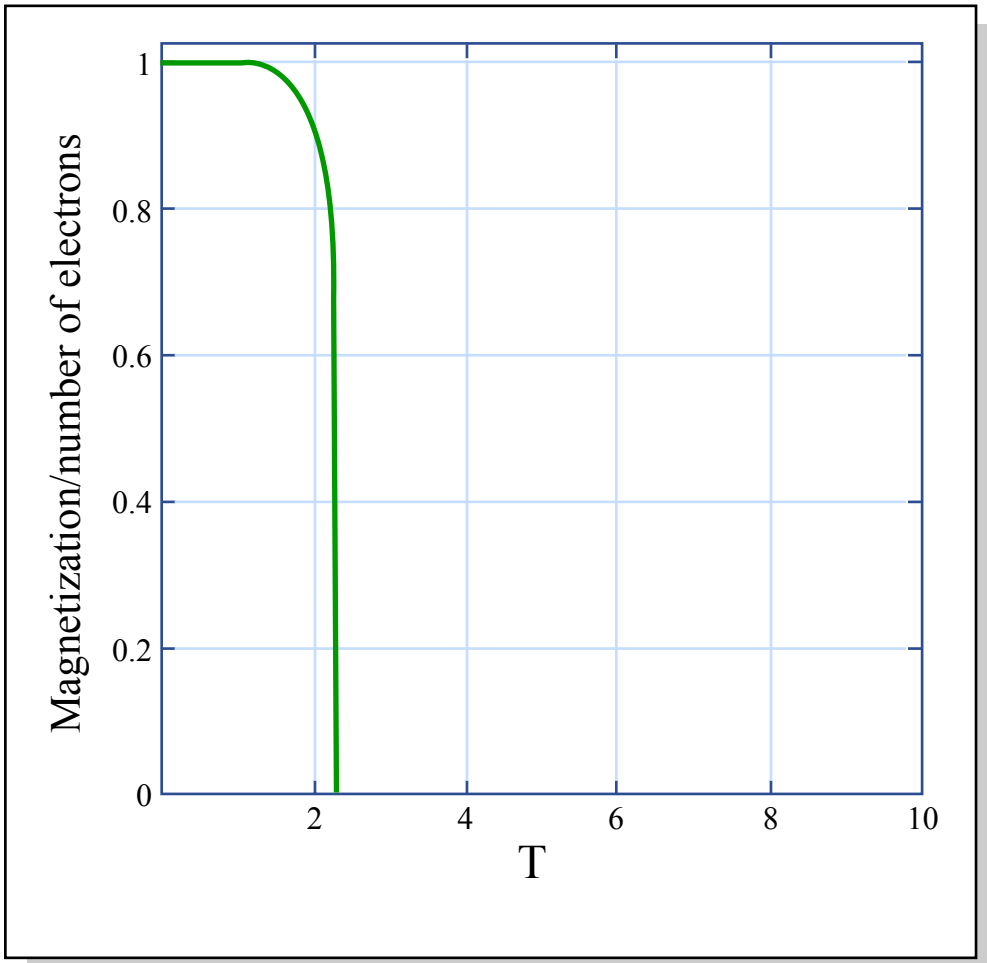
Image of Ernest Ising.

2D Ising-Lenz Results





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Simple sampling algorithm

1. $M=Z=0;\ k=1$
2. Pick a state (**s**) at random
3. Compute statistical weight $w_k=exp(-E(s)/T)$
4. $M_k=M(s);\ k=k+1$
5. If $k<k_{max}$ go to 2
6. $$\langle M \rangle = \sum_{k=1}^{k_{\max}} M_k w_k \Big/ \sum_{k=1}^{k_{\max}} w_k$$

Monte Carlo: Metropolis algorithm

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Nicolas Metropolis **Edward Teller** **Stanslaw Ulam**

Importance sampling algorithm

0. *M=Z=0; k=1*
1. Generate a state (**s**) with probability P(s)~exp(-E(s)/T).
2. $M_k=M(s)$; $k=k+1$
3. If $k<k_{max}$ go to 2
4. $$\langle M \rangle = \frac{1}{k_{\max}} \sum_{k=1}^{k_{\max}} M_k$$