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I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

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# COLLEGE ON MEDICAL PHYSICS

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# INTRODUCTION TO MONTE CARLO METHOD

H. A. Farach

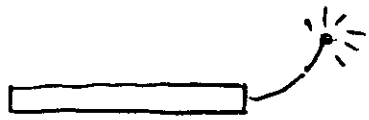
University of South Carolina
Columbia
USA

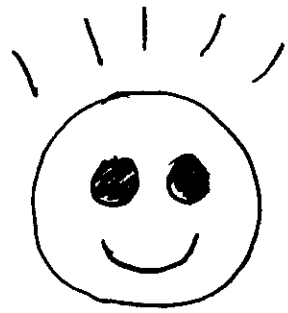
# Introduction to Monte Carlo Method

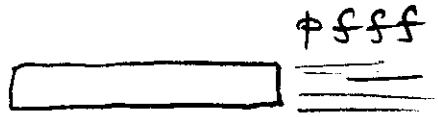
## and I mean INTRODUCTION

H.A. Farach
Dept. of Physics
Univ. South Carolina
Columbia S.C. 29208
USA

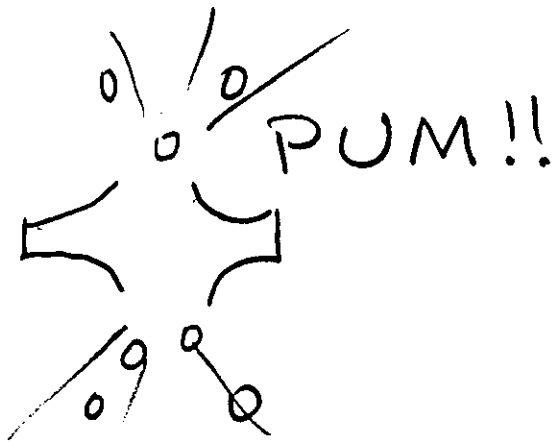
Before

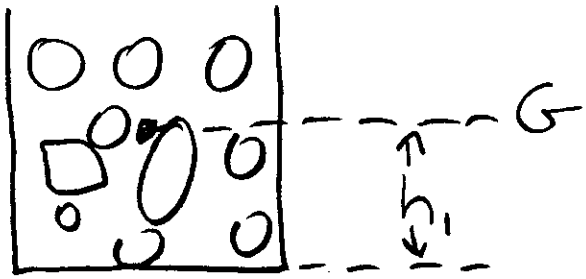


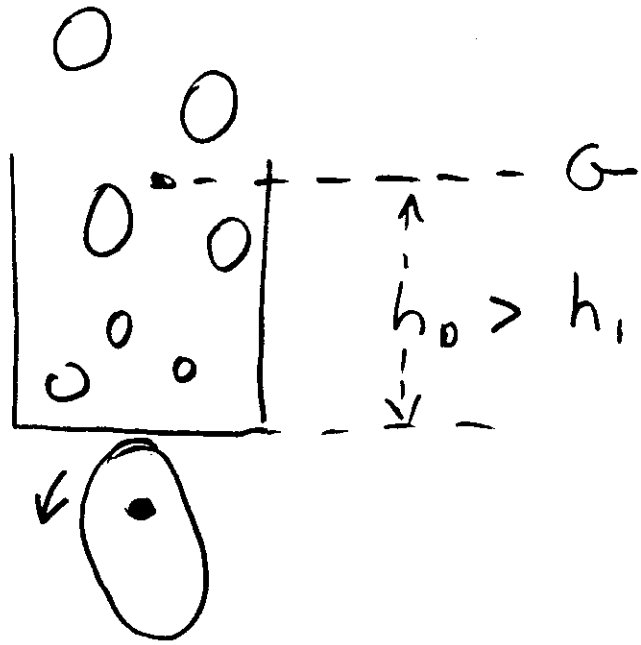


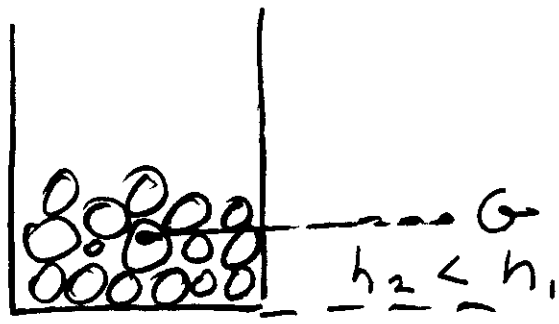


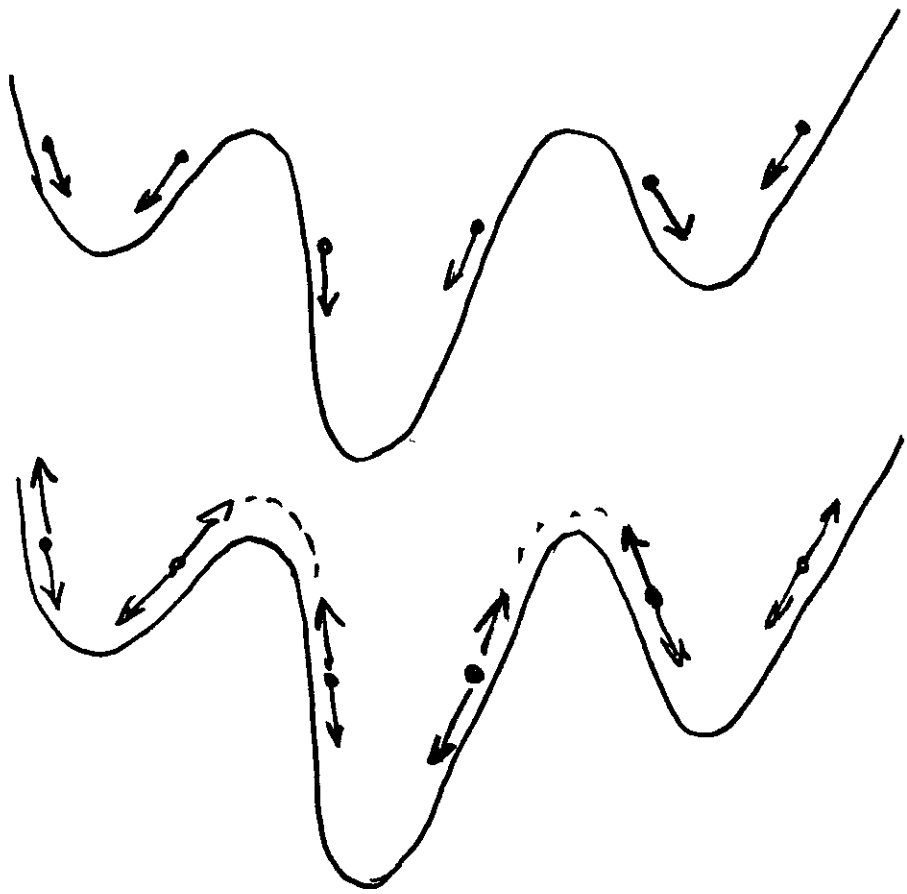

After

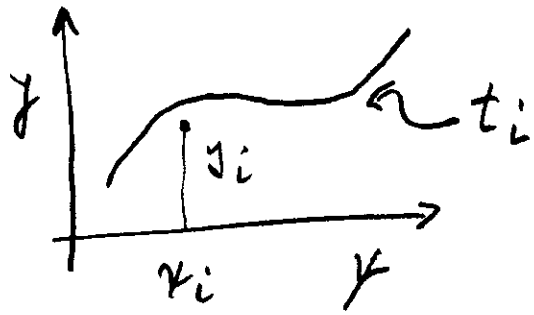





G
$h_1$


G
$h_0 > h_1$


G
$h_2 < h_1$

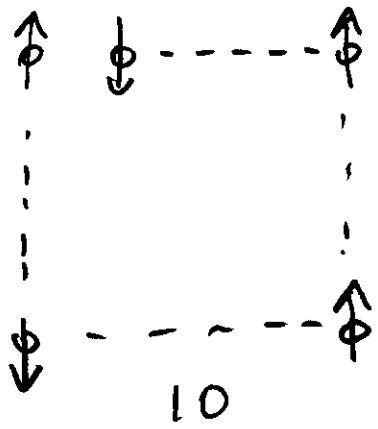





$$\psi \equiv \sum_i (t_i - y_i)^2$$

$$x_i \to x_i \pm \delta x_i \to \quad y_i \to y_i \pm \delta y_i$$

$$\psi \to \psi \pm \delta\psi$$




$S = 1/2$

$m_s = \pm 1/2$

$10 \times 10 = 100$ spins

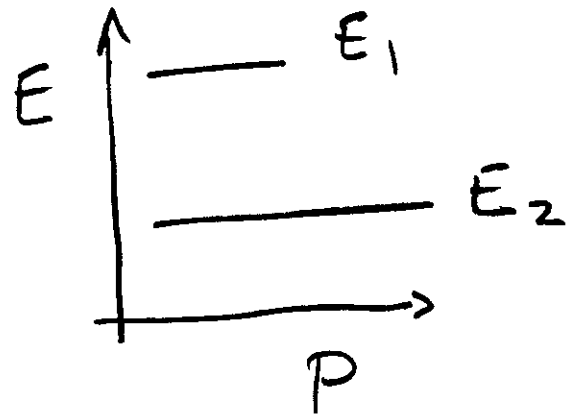
$n = \#$ of states $= 2^{100}$

$2^{100} \approx 10^{28}$

each calculation $t' = 10^{-6}$ s

$t = 10^{28} t' = 10^{22}$ s

$\cong 10^6$ life of the UNIVERSE!!




$$P_1(E_1) = C\, e^{-E_1/T}$$

$$P_2(E_2) = C\, e^{-E_2/T}$$

$$\overline{1} = C \sum_i e^{-E_i/T}$$

$$C = \frac{1}{\sum_i} = \frac{1}{Z}$$

$$Z = \sum_i e^{-E_i/T}$$ partition function

$$Pop_1(E_1) = N\, e^{-E_1/T} / Z$$

$$Pop_2(E_2) = N\, e^{-E_2/T} / Z$$

$$\frac{P_1(E_1)}{P_2(E_2)} = \frac{e^{-E_1/T}}{e^{-E_2/T}}$$

$$= \frac{e^{(-E_1+E_2)/T}}{1}$$

$$\frac{P_1}{P_2} = \frac{e^{-\Delta E/T}}{1}$$

Up with $P = e^{-\Delta E/T}$

Down with $P = 1$

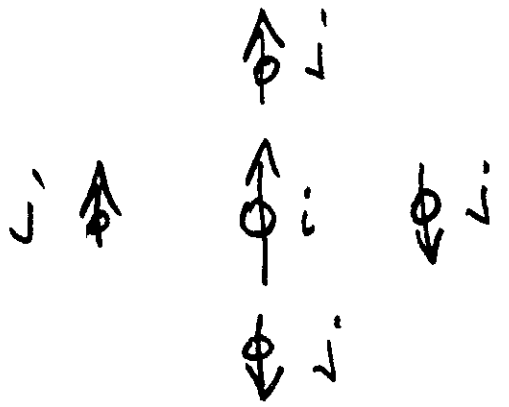
Normally $P_{up} = 0$

$P_{down} = 1$

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

$\sigma = \pm 1 \qquad J = 1$

$-J$ indicated ferromagnetic order




$E = -(-1 + 1 + 1 + 1) = -2 \qquad \sigma_i (+)$

$E = -(1 - 1 - 1 - 1) = 2 \qquad \sigma_i (-)$

Start $\sigma_i (-) \qquad E = +2$

if flip $\sigma_i (+) \qquad E = -2$

$$\Delta E = (-2) - (+2)$$

$$= -4$$

$\Delta E < 0$ ; down ; **flip**

Start $\sigma_i(+)$ $E = -2$

if flip $\sigma_i(-)$ $E = +2$

$$\Delta E = (+2) - (-2)$$

$$= +4$$

$\Delta E > 0$, up, flip with $P = e^{-\Delta E/T}$

how?

Call $r$ $0 \leq r \leq 1$

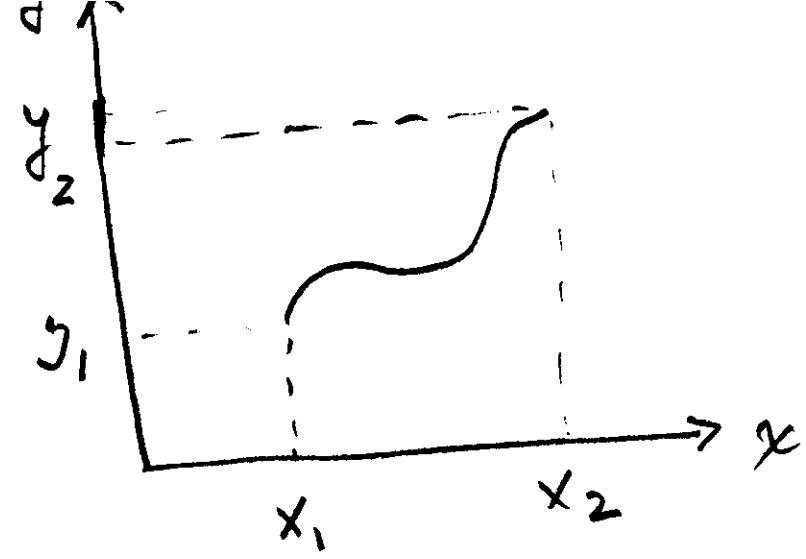
if $\Delta E \gg 0$ should be more difficult

if $\Delta E \gtrsim 0$ should be less difficult

for $\Delta E \gg 0$ $P = e^{-\Delta E/T} \to 0$

often $r > P$ so

**flip only when $P > r$**




$$I = \int_{x_1}^{x_2} y \, dx$$

Call $r_1$ $\quad x = (X_2 - X_1) * r_1 + X_1$

Calculate $y_c(x)$ Call $r_2$ $\quad y = (Y_2 - Y_1) * r_2 + Y_1$

| Col 1 | Col 2 |
|---|---|
| always | only if $y \le y_c$ |
| $N$ | $n$ |

$$I = \frac{n}{N} \times (Y_2 - Y_1)(X_2 - X_1)$$

$t\ (t_1, t_2 \ldots t_n)$

initial guess

$y\ (y_1, y_2 \ldots y_n)$

$$\psi = \sum_i (t_i - y_i)^2$$

change a parameter

$y \rightarrow y'$

$$\psi' = \sum_i (t_i - y_i')^2$$

$$\Delta\psi = \psi' - \psi$$

if $\Delta\psi < 0$ **flip**

if $\Delta\psi > 0$ flip with $P = e^{-\Delta\psi/T}$

— x —