

# Numerical Methods in Quantum Many-body Theory

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Ewha,  
Where Change Begins



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# Numerical Methods in Quantum Many-Body Theory

# Contents

- Introduction to Computational Physics
- Monte Carlo Methods: Basics and Applications
- Numerical Calculations in Quantum Theory of Many Particles
  - Example: Dynamical Mean-Field Theory



# Introduction to Computational Physics

# Computational Physics

What does atomic physics do?

Atoms, Molecules

What does nuclear physics do?

Nuclei

What does computational physics do?

Computers(?), Computation(?)

Physics



*Let's play with computers.*

*Let's play with physics.*

*Be Friends with computers*

# Steps in numerical works

1. Setting up a problem
2. Coding and running a program
3. Analyzing and visualizing results

# 1. Setting up a problem

- State and understand a problem
- Find relevant variables and how to solve it
- Convert it to a **computer-friendly** form

## 2. Coding and running a program

- Design a global structure
- Writing a program (Coding)
  - **Use**
    - pseudocode first
    - verified existing routine
    - separated logic groups
    - "comments"
  - **Avoid**
    - complex logic
    - tricky technique
    - computer-dependent language
  - Leave a **backup-copy** of programs before significant changes are made

## 2. Coding and running a program

- Testing and debugging a program
  - **Grammatical error**  
debugging at the compiler stage
  - **Terminated without results**  
infinite loops, memory access error, . . .
  - **Running but wrong results**  
???

# How to debug

- Working like a detective!!!
- Check global logic
- Check local logic by simulating a program personally
- Check line-by-line values of variables

# How to test results

- Check the result of the current program in the known special cases
- Check whether the current program reproduce other previous results
- Check whether the results are physically sensible

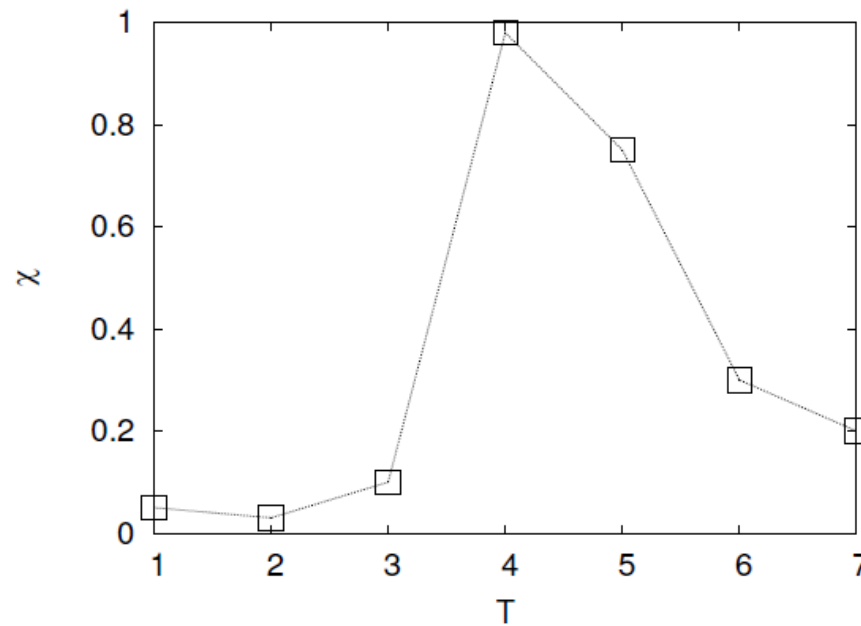
# 3. Analyzing & visualizing results

- Analysis of results are very important since it lays physical meaning on the results.
- Significance of the results is not given by how difficult the computation is but by how important its physical meaning is.
- Visualization helps us to understand results.
- It can emphasize the significance of results.

# 3. Analyzing & visualizing results

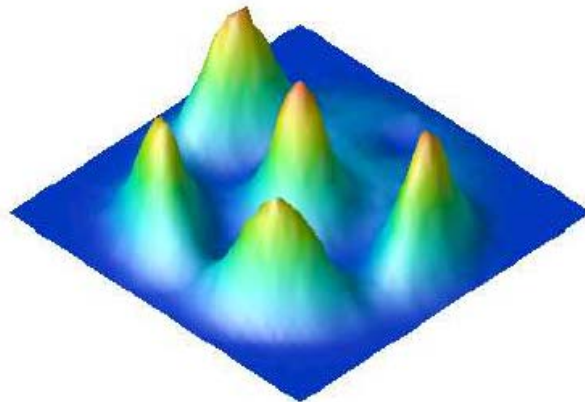
- Example

$T$	1	2	3	4	5	6	7
$\chi$	0.05	0.03	0.1	0.98	0.75	0.30	0.20

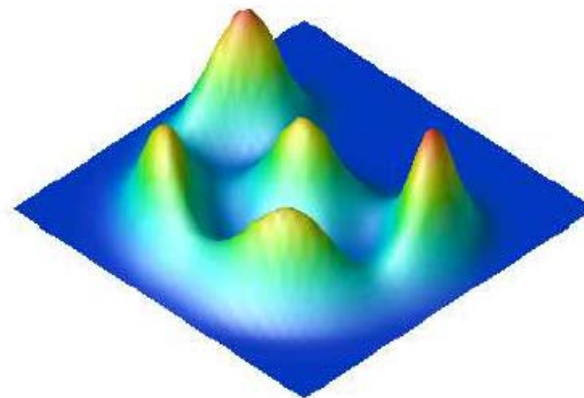


# 3. Analyzing & visualizing results

- Example



Exact



Our model

# Remark

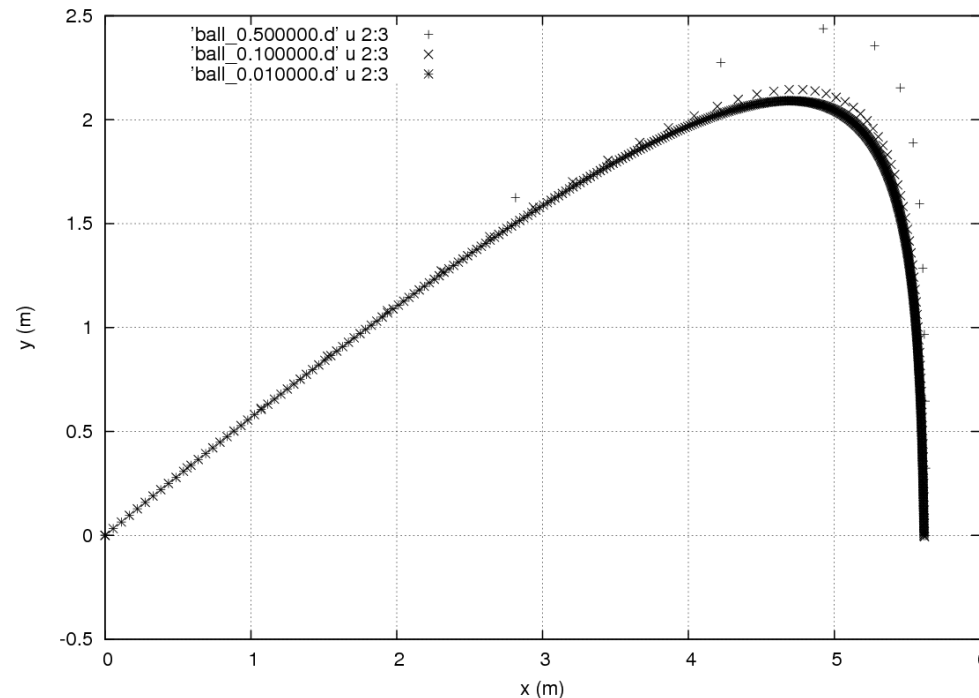
- Think in a way that computers do.
- Computers can perform numerical calculation very fast.
- Computers do not know physics, nor even have common senses.
- Understand how computer works as much as possible.
- *Let's play with computers.*

# Example: Throwing a ball through air

We throw a ball with the initial velocity  $v_0$  and the angle  $\theta_0$ . Then the ball is moving according to Newton equations:

$$m = 1.0 \text{ kg}, g = 9.8 \text{ m/s}^2, b = 3.9 \text{ kg/s}, v_0 = 25 \text{ m/s}, \text{ and } \theta_0 = \pi/6.$$

$$m \frac{d^2x}{dt^2} = -bv_x,$$
$$m \frac{d^2y}{dt^2} = -mg - bv_y,$$



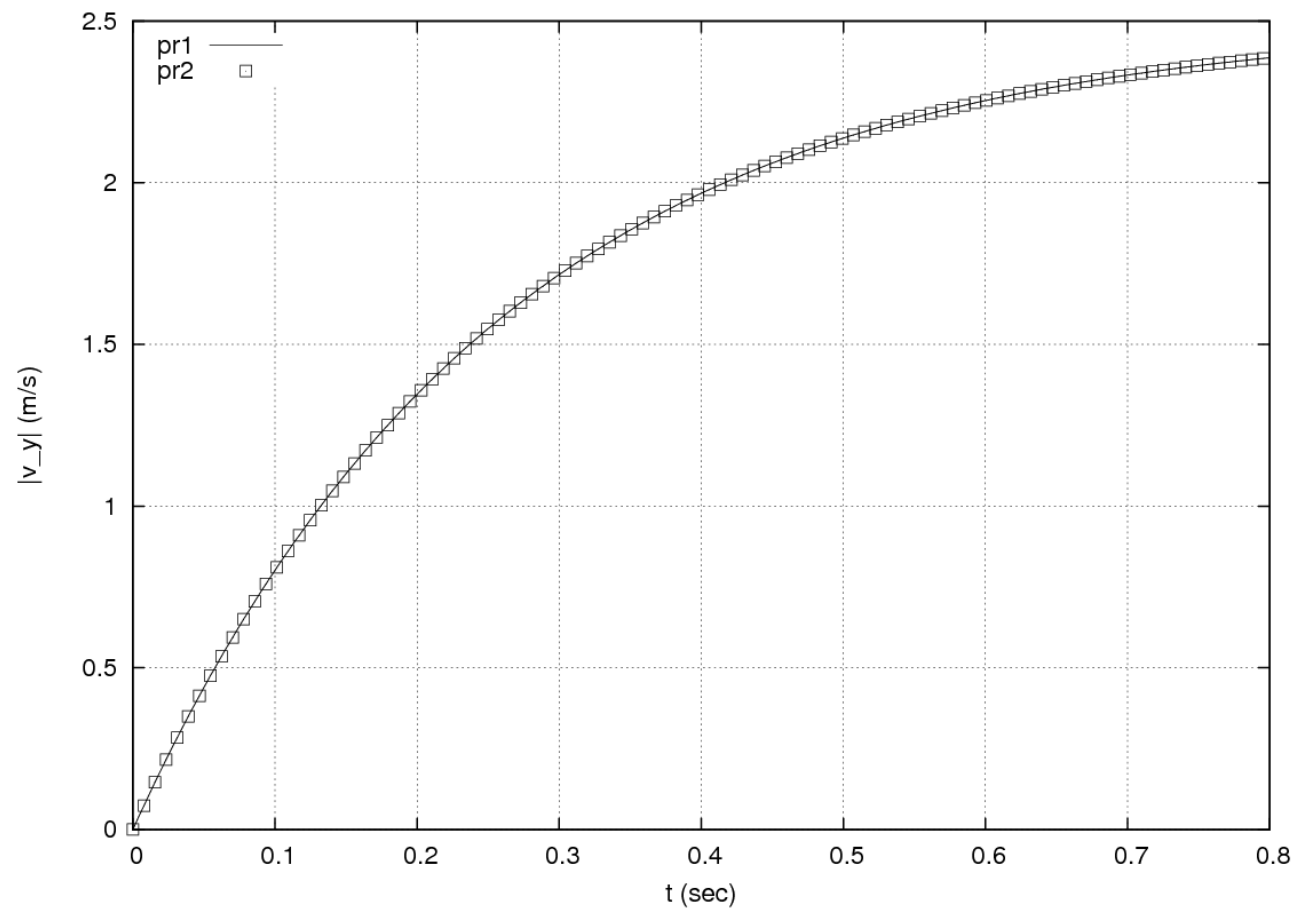
How do we know if the result is correct?

# How to test results

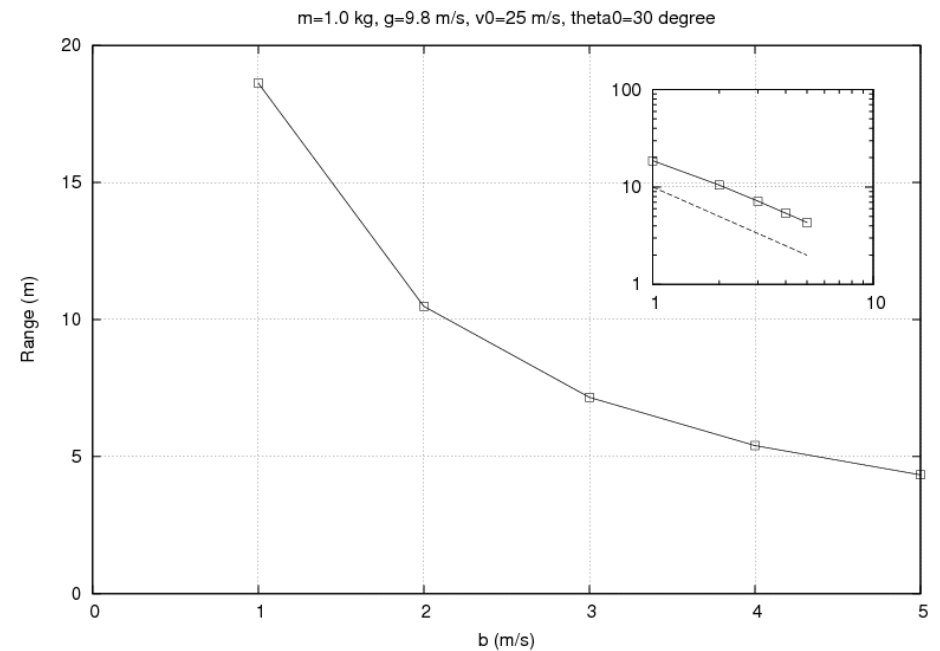
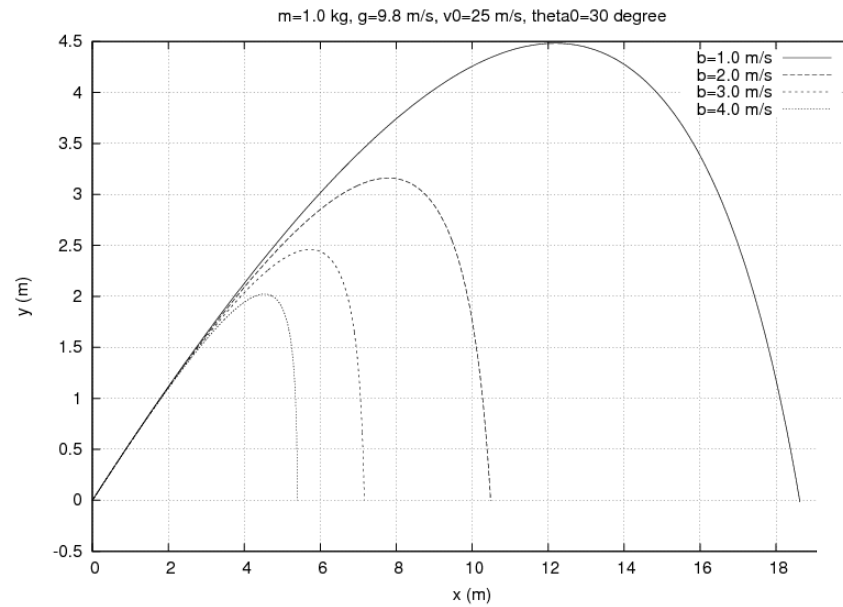
- Check special cases
- Check whether other previous results are reproduced
- Check whether the results are physically sensible

# Compare previous results

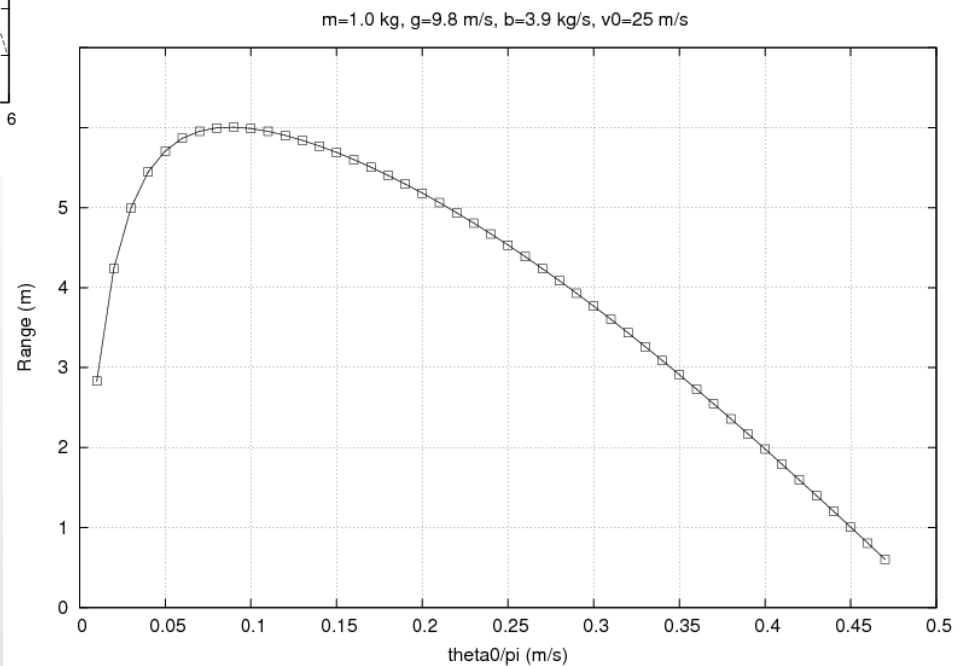
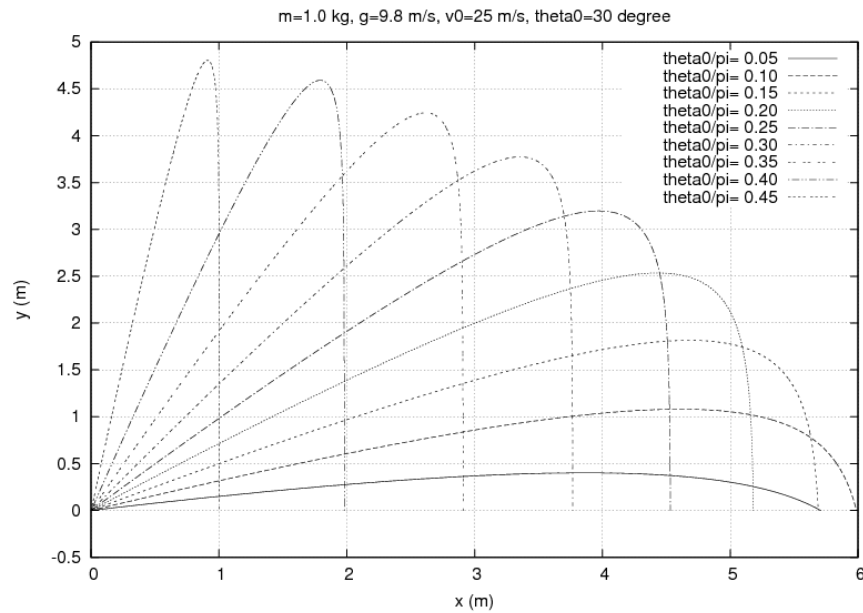
$$v_{x0} = 0, v_{y0} = 0$$



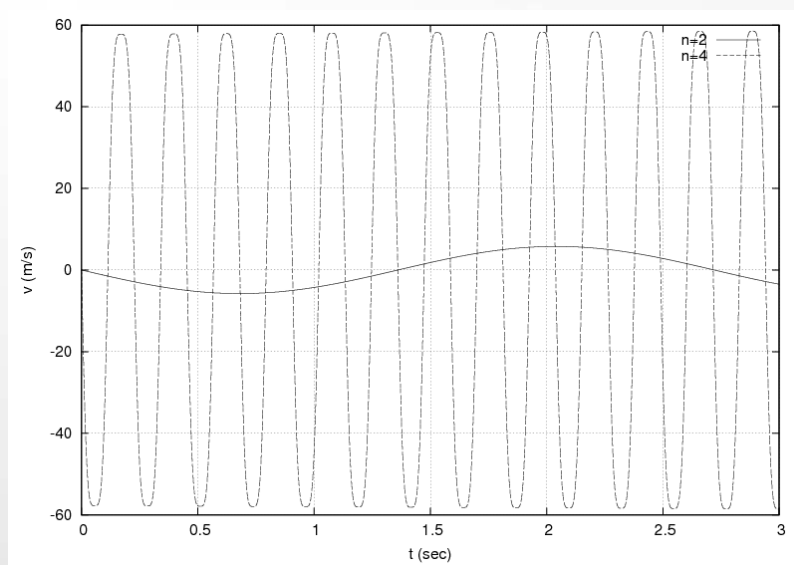
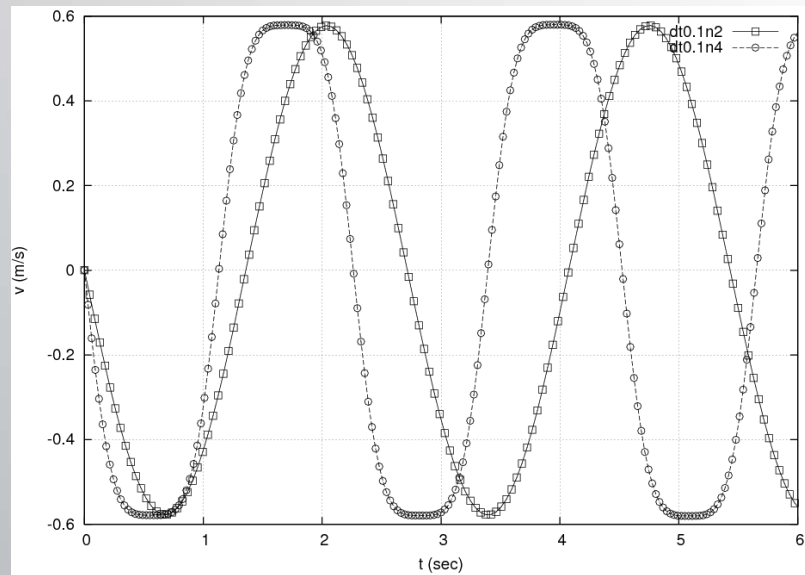
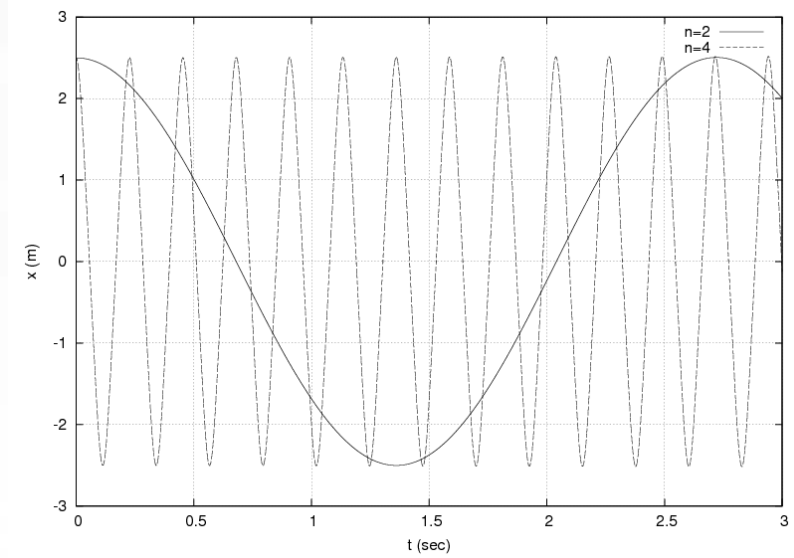
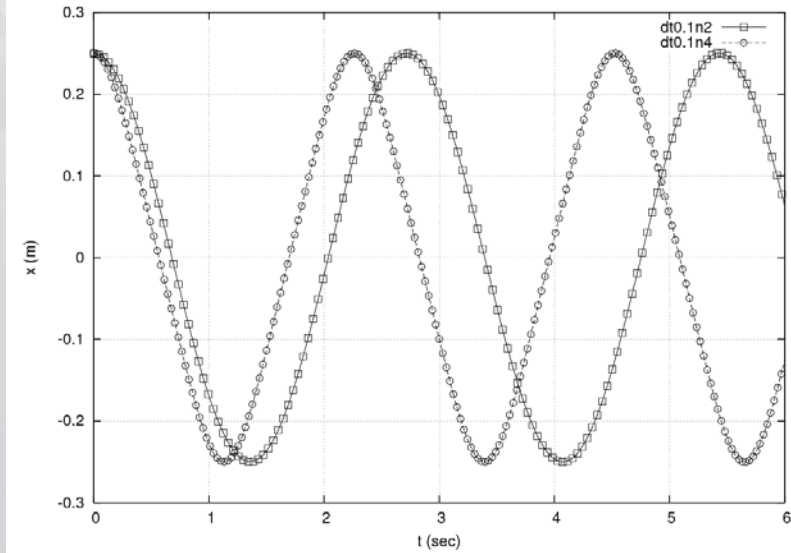
# Let's play with physics - variation of $b$



# Let's play with physics - variation of angle



# Let's play with physics

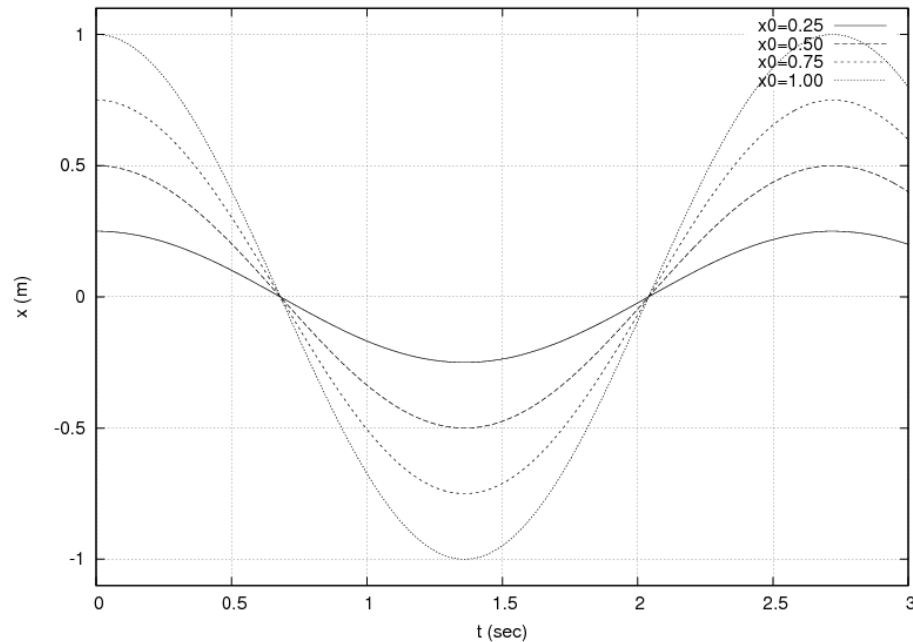


# Let's play with physics

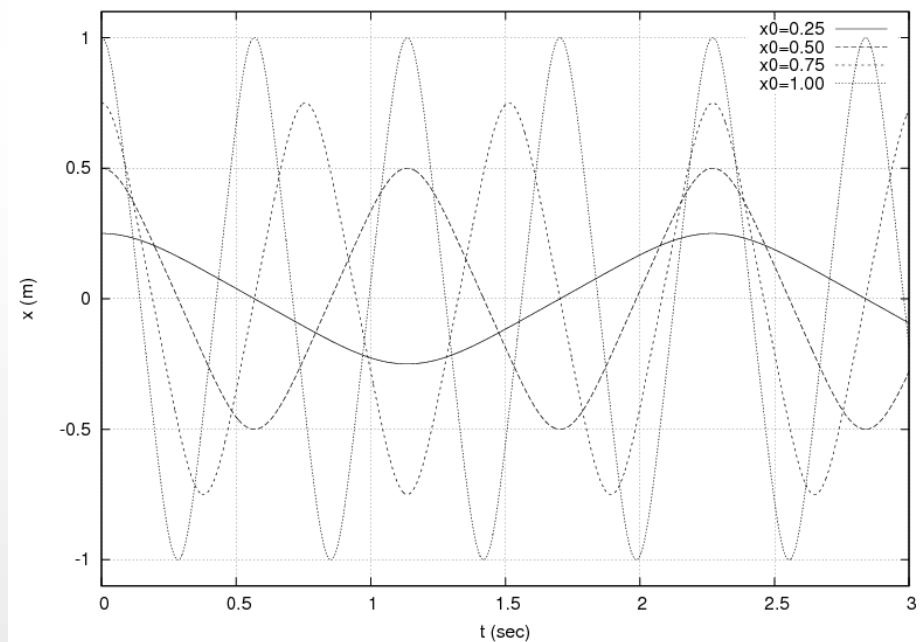
A particle is moving in a potential  $V(x) = ka \left(\frac{x}{a}\right)^n$ . Its motion is described by Newton equation

$$m \frac{d^2x}{dt^2} = -nk \left(\frac{x}{a}\right)^{n-1}.$$

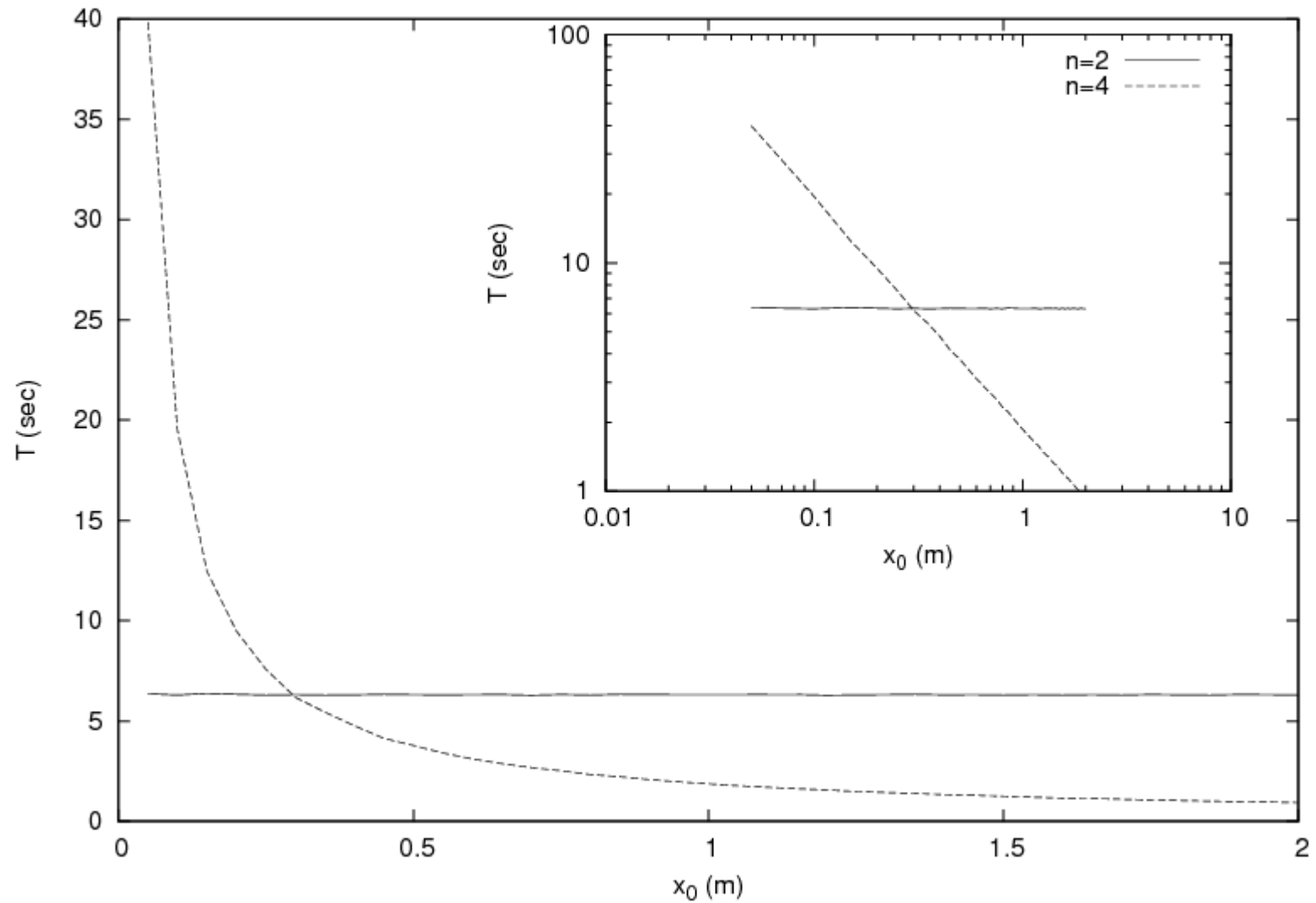
$n=2$



$n=4$



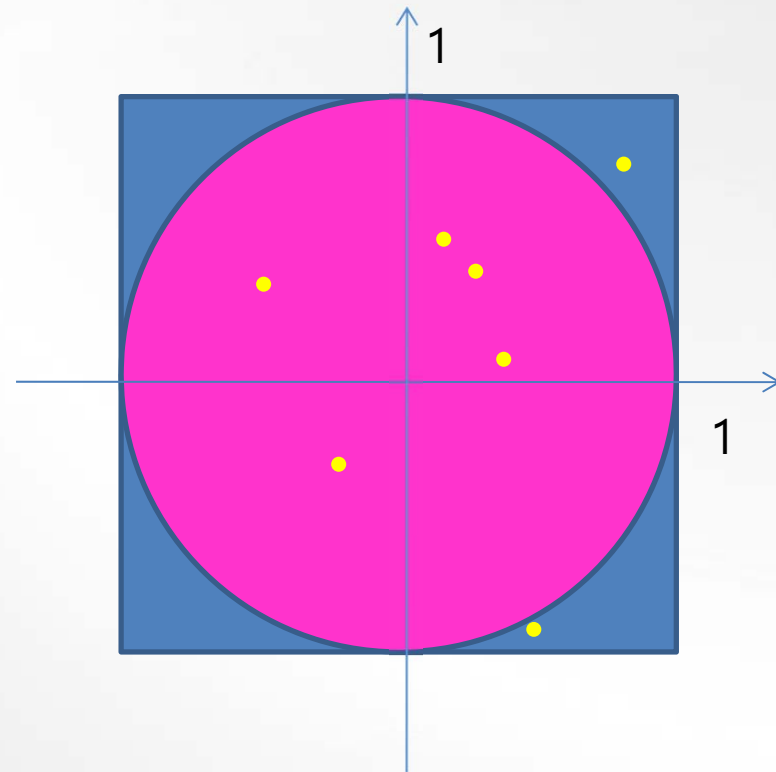
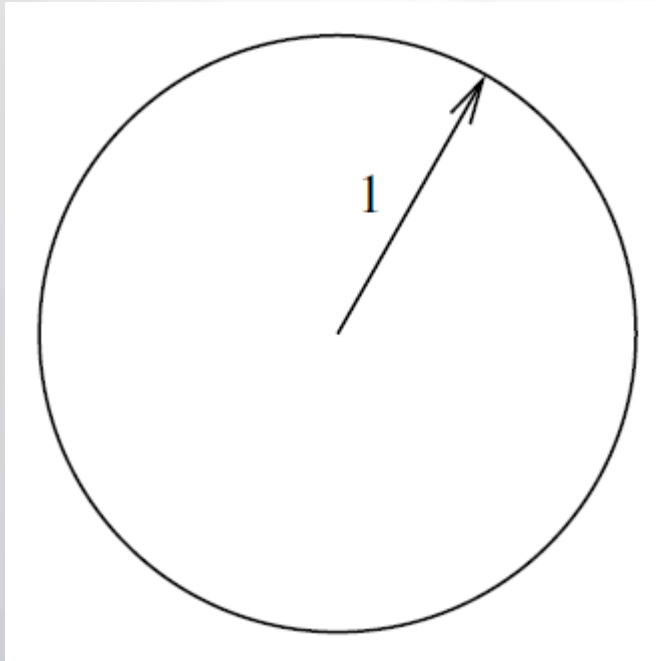
# Let's play with physics





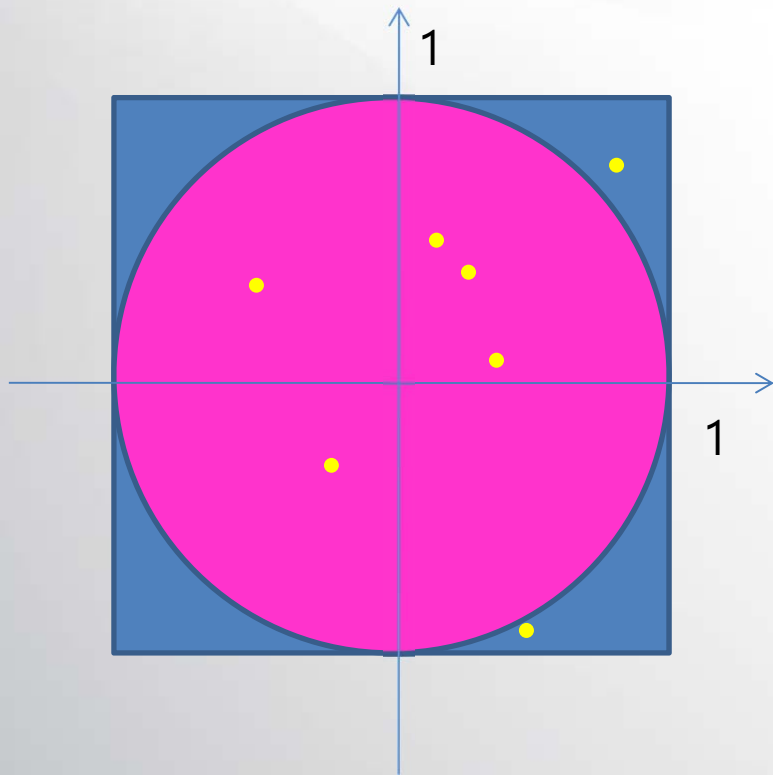
# Monte Carlo Methods: Basics and Applications

# Area of a circle



$$\text{Area} \approx 4 \times \left(\frac{5}{7}\right) \approx 2.9$$

# Area of a circle



pick up  $(x_i, y_i)$  randomly

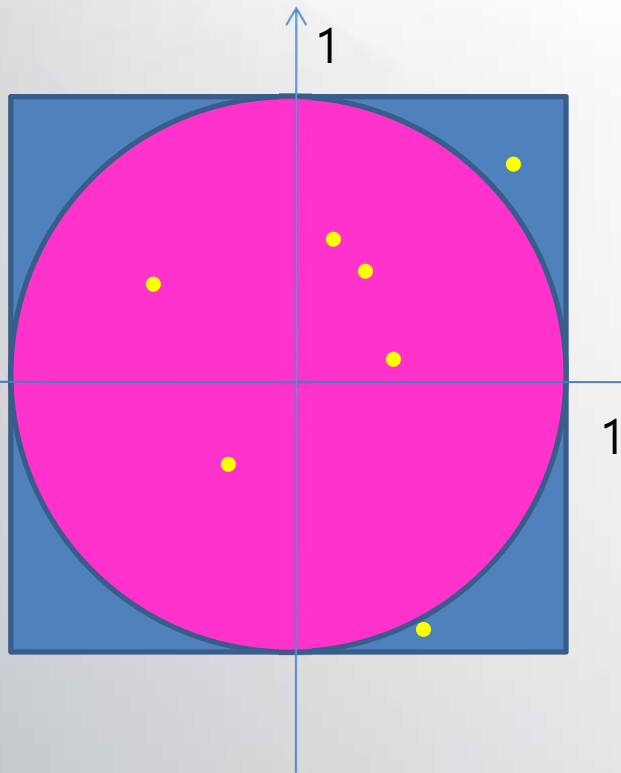
$$-1 \leq x_i \leq 1, -1 \leq y_i \leq 1$$

Area of a circle

$$\approx \frac{N(\sqrt{x^2 + y^2} < 1)}{N_{\text{total}}}$$

× Area of a square

# Area of a circle

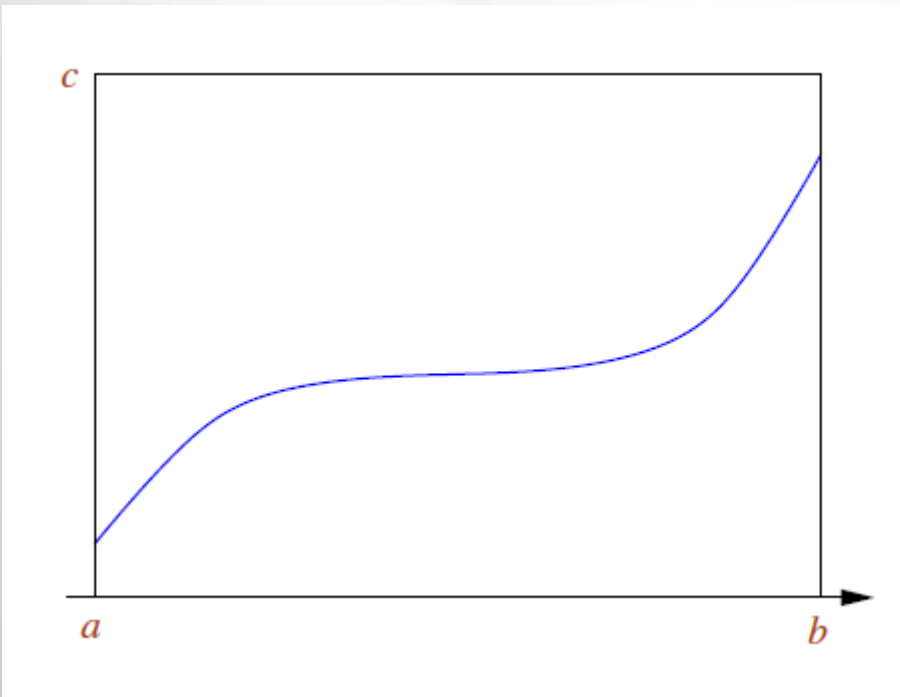


$N_{\text{tot}}$	1	2	3	4	area
10	9	8	8	7	3.200 $\pm 0.283$
100	83	86	84	80	3.330 $\pm 0.087$
1000	787	788	788	802	3.165 $\pm 0.025$
10000	7750	7824	7855	7861	3.129 $\pm 0.018$
100000	78619	78426	78380	78414	3.138 $\pm 0.004$
1000000	786076	785103	785503	785084	3.142 $\pm 0.002$

Area =

3.1415926535897932384626433832795028841971693993...

# Integration by Monte Carlo



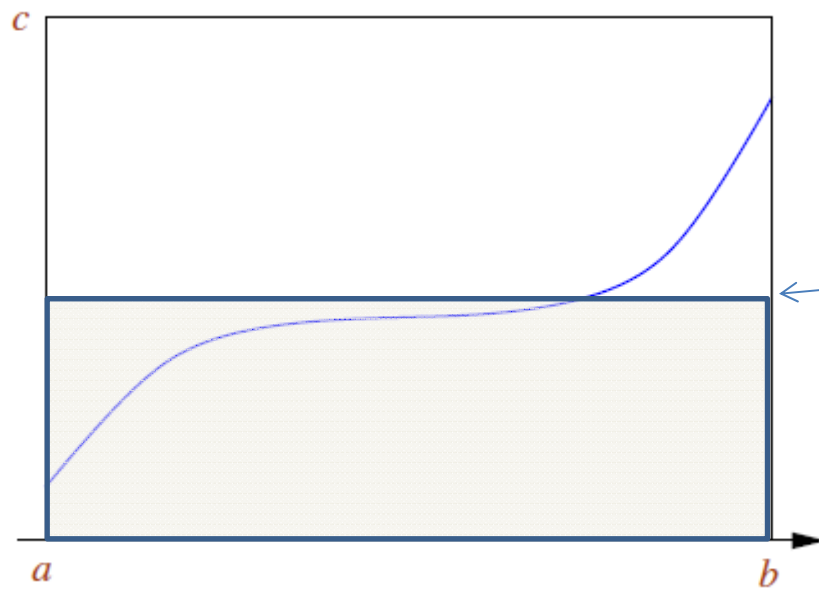
pick up  $(x_i, y_i)$  randomly

$$a \leq x_i \leq b, 0 \leq y_i \leq c$$

$$\int_a^b f(x) dx$$

$$\approx \frac{N(y_i < f(x_i))}{N_{\text{total}}} \times c(b - a)$$

# Simple Sampling

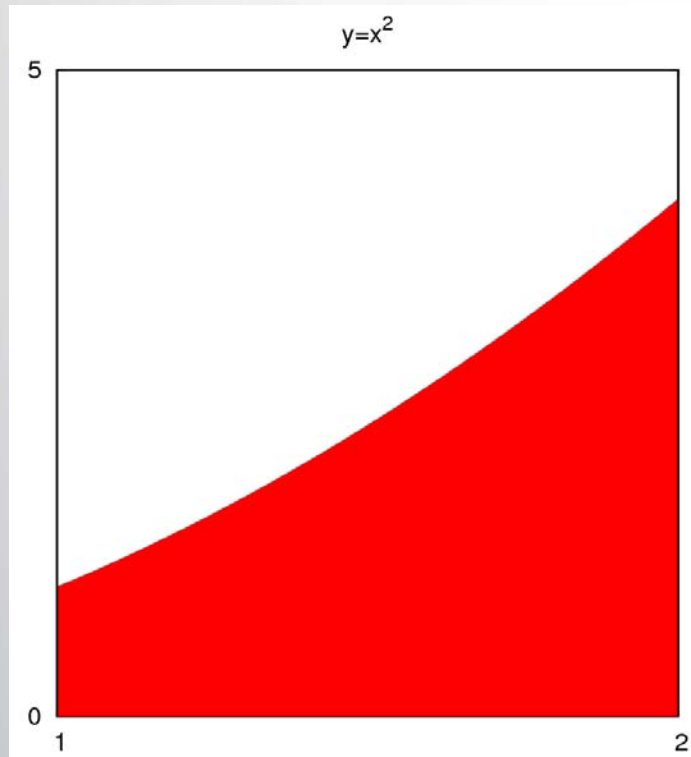


Pick up  $x_i$  randomly for  $a \leq x_i \leq b$

$$\frac{1}{b-a} \int_a^b f(x) dx \approx \frac{1}{N} \sum_i f(x_i)$$

# Simple Sampling

$$\int_1^2 x^2 dx$$



$N_{\text{tot}}$	Method I	Simple Sampling
10	$2.250 \pm 0.433$	$2.238 \pm 0.202$
100	$2.462 \pm 0.329$	$2.339 \pm 0.051$
1000	$2.336 \pm 0.044$	$2.323 \pm 0.031$
10000	$2.324 \pm 0.012$	$2.339 \pm 0.009$
100000	$2.334 \pm 0.007$	$2.334 \pm 0.002$
1000000	$2.335 \pm 0.002$	$2.333 \pm 0.001$

# Importance Sampling

Pick up  $x_i$  with probability  $p(x_i)$  for  $a \leq x_i \leq b$

$$\int_a^b f(x) dx \approx \frac{1}{N} \sum_i f(x_i) p^{-1}(x_i)$$

$$\int_a^b g(x) p(x) dx \approx \frac{1}{N} \sum_i g(x_i)$$

Note  $\int_a^b p(x) dx = 1$

# Simple versus Importance Sampling

$$I = \int_0^{100} x e^{-x} dx$$

- Simple sampling  
with  $f(x) = x e^{-x}$
- Importance sampling  
with  $f(x) = x$  and  $p(x) = e^{-x}$

$N_{\text{tot}}$	Simple Sampling	Importance Sampling
10	$0.4805 \pm 0.8272$	$0.8841 \pm 0.2106$
100	$0.9326 \pm 0.5208$	$0.9789 \pm 0.0325$
1000	$0.9078 \pm 0.1020$	$0.9884 \pm 0.0334$
10000	$0.9539 \pm 0.0607$	$1.0022 \pm 0.0115$
100000	$1.0000 \pm 0.0061$	$1.0002 \pm 0.0011$
1000000	$0.9981 \pm 0.0037$	$0.9998 \pm 0.0007$

# Metropolis Method

master equation

$$\frac{\partial P_n(t)}{\partial t} = \sum_{m(\neq n)} [P_m(t)W_{m \rightarrow n} - P_n(t)W_{n \rightarrow m}]$$

$P_n(t)$  : probability that the system is in state  $n$  at time  $t$

$W_{n \rightarrow m}$  : transition rate for  $n \rightarrow m$

In equilibrium 
$$\frac{\partial P_n(t)}{\partial t} = 0$$

detailed balance

$$P_m(t)W_{m \rightarrow n} = P_n(t)W_{n \rightarrow m}$$

From detailed balance 
$$\frac{W_{n \rightarrow m}}{W_{m \rightarrow n}} = \frac{P_m}{P_n}$$

In Metropolis method, we take 
$$W_{n \rightarrow m} = \min \left[ \frac{P_m}{P_n}, 1 \right]$$

# Metropolis Method (Cont'd)

$$I = \int_a^b f(x)p(x)dx$$

with probability  $p(x)$

1. Choose an initial value  $x=x_0$  as a uniform random number in the interval  $a \leq x_0 \leq b$ .
2. Repeat following steps and take the average of  $f(x)$  obtained in each repetition.
  - (a) Choose a trial value  $x^*$  as a uniform random number in the interval  $a \leq x^* \leq b$ .
  - (b) If  $p(x^*) > p(x)$ , set  $x = x^*$  since  $p(x^*)/p(x) > 1$ .
  - (c) If  $p(x^*) < p(x)$ , set  $x = x^*$  for a probability  $p(x^*)/p(x)$ .  
( Generate a uniform random number  $r$  ( $0 \leq r < 1$ ) and set  $x = x^*$  if  $r < p(x^*)/p(x)$ . )

# Example: Metropolis Method

ex)  $I = \int_0^{100} x^2 e^{-x} dx$  probability  $p(x) = e^{-x}$

1. Choose an initial value  $x=x_0$  as a uniform random number in the interval  $0 \leq x_0 \leq 100$ .
2. Repeat following steps and take the average of  $f(x) = x^2$  obtained in each repetition.
  - (a) Choose a trial value  $x^*$  as a uniform random number in the interval  $0 \leq x^* \leq 100$ .
  - (b) If  $p(x^*) > p(x)$  i.e.  $x^* < x$ , set  $x = x^*$  since  $p(x^*)/p(x) > 1$ .
  - (c) If  $p(x^*) < p(x)$  i.e.  $x^* > x$ , set  $x = x^*$  for a probability  $p(x^*)/p(x)$ .  
(Generate a random number  $r$  ( $0 \leq r < 1$ ) and set  $x = x^*$  if  $r < e^{x-x^*}$ .)

# Alternative Way for Metropolis Method

- When we take a trial value  $x^*$  [Step 2(a)], we use a following way
  1. Generate an increment value  $\Delta x$  as a uniform random number in the interval  $-R \leq \Delta x \leq R$ .
  2. Choose a trial value  $x^* = x + \Delta x$ .
- $$\text{acceptance ratio} \equiv \frac{\text{number of accepted steps}}{\text{number of total steps}}$$
- The recommended acceptance ratio is 0.5, which is known to guarantee faster convergence of Monte Carlo average.

# Metropolis Method for Multi-Dimension Integral

$$I = \prod_{i=1}^N \int dx_i f(x_1, \dots, x_N) p(x_1, \dots, x_N)$$

1. Choose initial values  $\{x_i^{(0)}\}$  randomly.
2. Determine  $i$  randomly ( $i = 1, 2, \dots, N$ ).
3. Choose a trial value  $x^*$  randomly.
4. If  $p(x^*) > p(x_i)$ , set  $x_i = x^*$  since  $p(x^*)/p(x_i) > 1$ .
5. If  $p(x^*) < p(x_i)$ , set  $x_i = x^*$  for a probability  $p(x^*)/p(x_i)$ .  
(Generate a random number  $r$  ( $0 \leq r < 1$ ) and set  $x_i = x^*$  if  $r < p(x^*)/p(x_i)$ .)
6. Repeat 2 to 5  $N$  times.
7. Take the average of  $f(x_1, \dots, x_N)$ .
8. Repeat 2 to 7.

# Statistical Mechanics of Thermodynamic Systems

- partition function

$$Z = \sum_s e^{-E_s/k_B T}$$

- physical quantity

$$\langle O \rangle = \sum_s O_s P_s$$

with the probability

$$P_s = \frac{1}{Z} e^{-E_s/k_B T}$$

- appropriate problem to use the importance sampling with probability  $P_s$

# Metropolis method

From detailed balance

$$\frac{W_{n \rightarrow m}}{W_{m \rightarrow n}} = \frac{P_m(t)}{P_n(t)} = e^{-\Delta E/k_B T}$$

with  $\Delta E = E_m - E_n$

We will set

$$W_{n \rightarrow m} = \begin{cases} e^{-\Delta E/k_B T} & \Delta E > 0 \\ 1 & \Delta E < 0 \end{cases}$$

# Ensemble average

In each step

calculate physical quantity  $O_s$

and take an arithmetic average

$$\langle O \rangle = \frac{1}{N} \sum_s O_s$$

Perform the calculation even at **rejected** steps.

# Metropolis importance sampling with Ising spins

1. Choose an initial state randomly.

$$\sigma_1 = +1, \sigma_2 = -1, \sigma_3 = -1, \dots, \sigma_N = 1$$

2. Choose site  $i$  randomly.

3. Calculate  $\Delta E$  for spin flip at site  $i$ .

$$\Delta E = E(\sigma_1, \dots, -\sigma_i, \dots, \sigma_N) - E(\sigma_1, \dots, +\sigma_i, \dots, \sigma_N)$$

4. i) If  $\Delta E < 0$ , flip the spin

- ii) If  $\Delta E > 0$ ,

generate a random number  $r$  such that  $0 < r < 1$

and flip the spin only if  $r < \exp(-\Delta E/k_B T)$ .

5. Repeat steps 2, 3, 4.

# Simple example

$N$  noninteracting Ising spins in an external magnetic field  $H$

$$\mathcal{H} = -H \sum_i \sigma_i \quad (\sigma_i = \pm 1)$$

partition function

$$\begin{aligned} Z &= \sum_{\sigma_1=-1}^1 \sum_{\sigma_2=-1}^1 \dots \sum_{\sigma_N=-1}^1 e^{-\mathcal{H}/k_B T} \\ &= \left( \sum_{\sigma_1=-1}^1 e^{H\sigma_1/k_B T} \right) \left( \sum_{\sigma_2=-1}^1 e^{H\sigma_2/k_B T} \right) \dots \left( \sum_{\sigma_N=-1}^1 e^{H\sigma_N/k_B T} \right) \\ &= \left( e^{-H/k_B T} + e^{H/k_B T} \right)^N \end{aligned}$$

# Simple example (cont'd)

free energy

$$F = -k_B T \ln Z = -k_B T N \ln(e^{-H/k_B T} + e^{H/k_B T})$$

magnetization

$$m = -\frac{\partial f}{\partial H} = \tanh(H/k_B T)$$

susceptibility

$$\chi = \frac{\partial m}{\partial H} = \frac{1}{k_B T} \operatorname{sech}^2(H/k_B T)$$

internal energy

$$\frac{U}{N} = -\frac{1}{N} \frac{\partial}{\partial \beta} \ln Z = -H \tanh(H/k_B T)$$

# Metropolis importance sampling (simple example)

1. Choose an initial state randomly.

$$\sigma_1 = +1, \sigma_2 = -1, \sigma_3 = -1, \dots, \sigma_N = 1$$

2. Choose site  $i$  randomly.
3. Calculate  $\Delta E$  for spin flip at site  $i$ .

$$\Delta E = 2H\sigma_i$$

4. i) If  $2H\sigma_i < 0$ , set  $\sigma_i = -\sigma_i$   
ii) If  $2H\sigma_i > 0$ ,  
generate a random number  $r$  such that  $0 < r < 1$   
and set  $\sigma_i = -\sigma_i$  only if  $r < \exp(-2H\sigma_i/k_B T)$ .
5. Repeat steps 2, 3, 4.

# Some Useful Tips

1. We have to allow several equilibration time before averaging physical quantities.

2. When we calculate  $\Delta E$ ,

in most cases we need not evaluate  $E_{\text{initial}}$  and  $E_{\text{trial}}$  separately.

ex) noninteracting spins

$$\Delta E = E_{\text{trial}} - E_{\text{initial}} = -H(\sigma_i^{\text{trial}} - \sigma_i^{\text{initial}})$$

3. When we calculate physical quantities,

we can just update each quantity only at accepted steps.

ex)  $E^{\text{final}} = E^{\text{initial}} + \Delta E$

$$M^{\text{final}} = M^{\text{initial}} + (\sigma_i^{\text{trial}} - \sigma_i^{\text{initial}})$$

# Some Useful Tips

4. To improve the calculation speed, reduce the number of complicated mathematical functions inside a micro Monte Carlo routine.

ex) We can store one parameter  $\exp(-H/k_B T)$  in a pre-defined variable.

5. Use dimensionless parameters. How do we deal with  $k_B$ ?

ex) i) Use  $T' \equiv k_B T / H$  for noninteracting spins

$T'$  is a temperature in units of  $H/k_B$ .

ii) Use  $T' \equiv k_B T / J$  for Ising spins with nearest-neighbor interactions

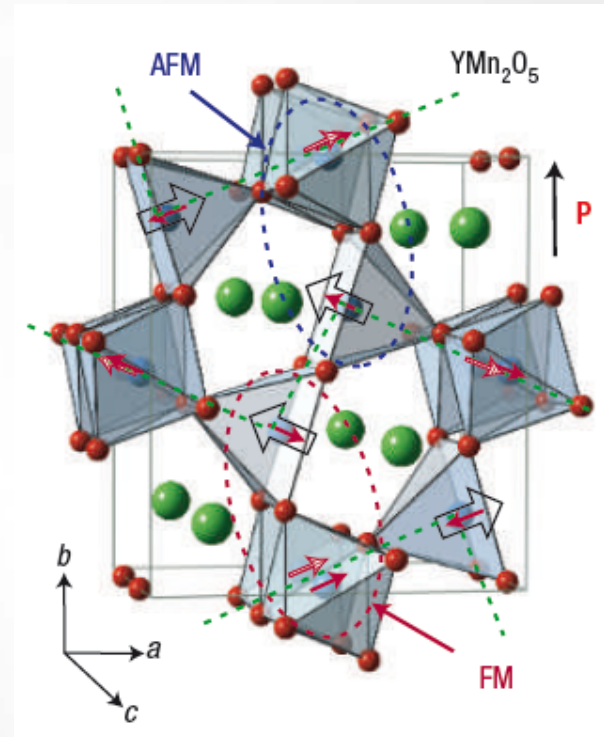
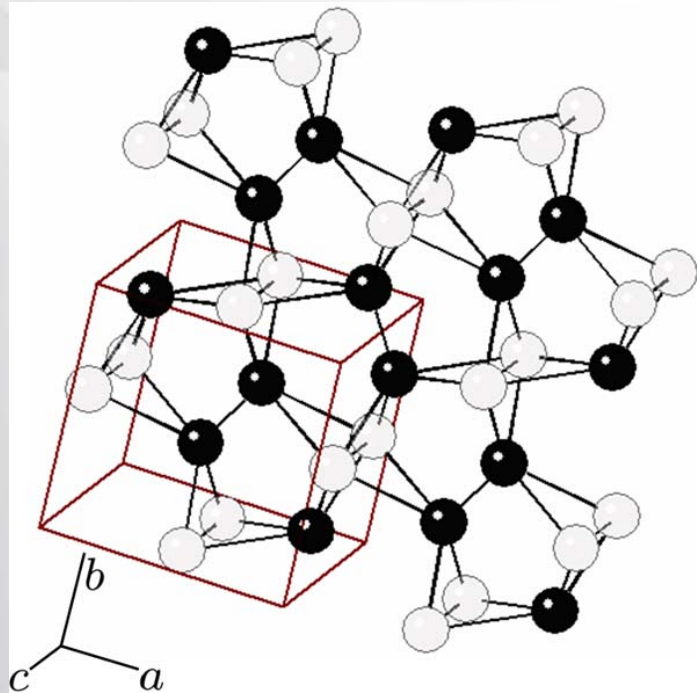
tions

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$



**Monte Carlo simulations:  
Multiferroic –  $\text{BiMn}_2\text{O}_5$**

# $\text{RMn}_2\text{O}_5$ (R=Tb, Y, Dy, Ho, Bi, ...)

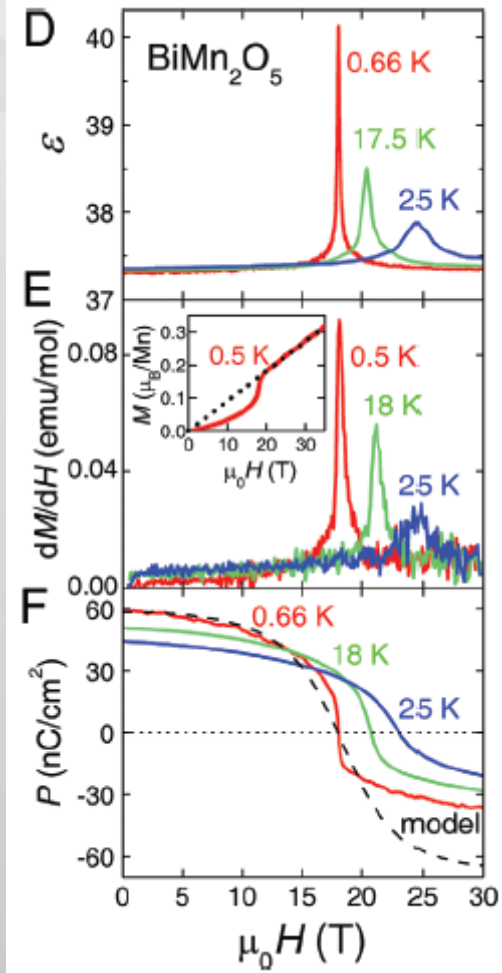


$\text{Mn}^{4+}$  : octahedrally coordinated ( $S=3/2$ )



$\text{Mn}^{3+}$  : tetrahedrally coordinated ( $S=2$ )

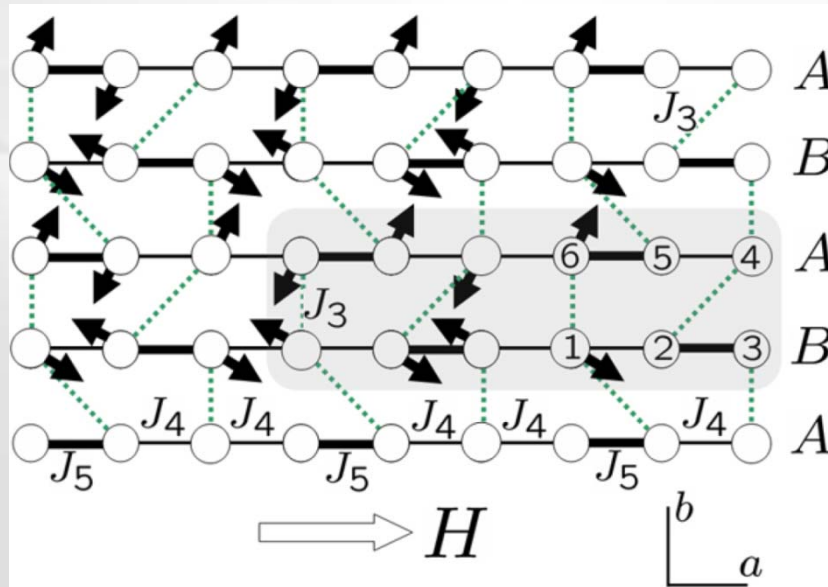
# BiMn<sub>2</sub>O<sub>5</sub>



- Application of high magnetic fields along the  $a$  axis
- Sharp symmetric peak in  $dM/dH$  and  $\varepsilon$  at low temperatures
- Abrupt sign change in  $P$

*Magnetic-field-induced metaelectric transition*

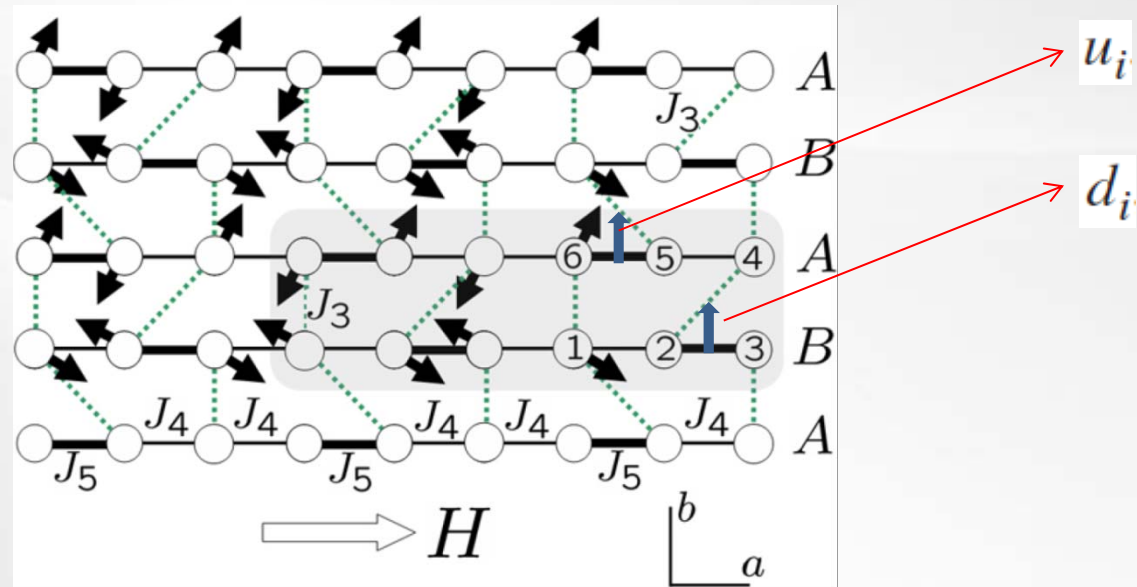
# Exchange interactions



$$J_3 \ll J_4, J_5$$

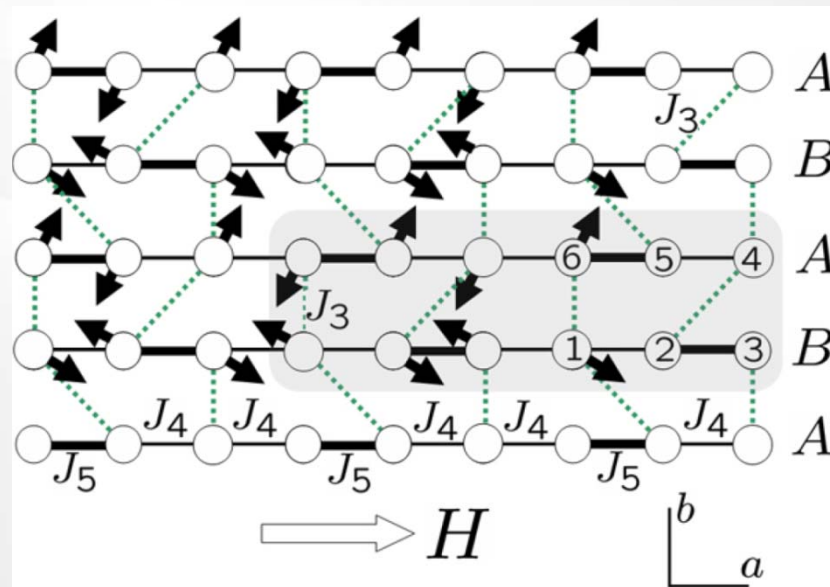
$$\begin{aligned}
 E_1 = & J_5 \sum_i (S_{i2} \cdot S_{i3} + S_{i5} \cdot S_{i6}) \\
 & + J_4 \sum_i (S_{i1} \cdot S_{i2} + S_{i4} \cdot S_{i5} + S_{i3} \cdot S_{i+\hat{x},1} + S_{i4} \cdot S_{i+\hat{x},6}), \\
 E_2 = & J_3 \sum_i (S_{i1} \cdot S_{i6} + S_{i2} \cdot S_{i4} + S_{i4} \cdot S_{i+\hat{y},3} + S_{i5} \cdot S_{i+\hat{y},1}),
 \end{aligned}$$

# Spin-lattice coupling via exchange striction



$$\begin{aligned}
 E_3 = & \frac{1}{2\chi} \sum_i (d_i^2 + u_i^2) + \frac{1}{4} \gamma \sum_i (d_i^4 + u_i^4) \\
 & - \sum_i d_i (\mathbf{S}_{i3} \cdot \mathbf{S}_{i-\hat{y},4} - \mathbf{S}_{i2} \cdot \mathbf{S}_{i4}) \\
 & - \sum_i u_i (\mathbf{S}_{i1} \cdot \mathbf{S}_{i6} - \mathbf{S}_{i5} \cdot \mathbf{S}_{i+\hat{y},1}).
 \end{aligned}$$

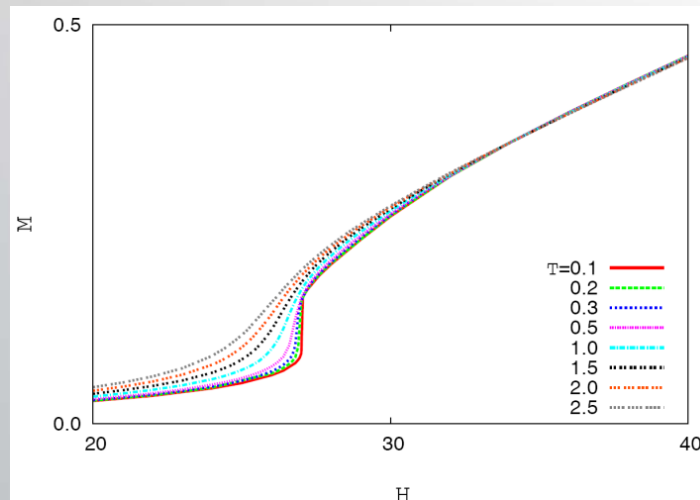
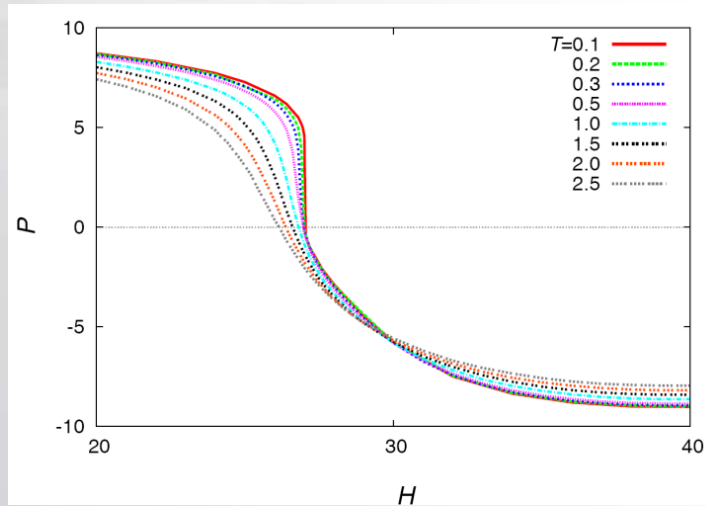
# Single-ion anisotropy + magnetic field



$$E_4 = -I \sum_i \sum_{\alpha=1}^3 (\mathbf{S}_{i\alpha} \cdot \hat{n}_A)^2 - I \sum_i \sum_{\alpha=4}^6 (\mathbf{S}_{i\alpha} \cdot \hat{n}_B)^2$$

$$E_5 = -H \sum_i \sum_{\alpha=1}^6 \mathbf{S}_{i\alpha} \cdot \hat{x}$$

# Polarization and Magnetization

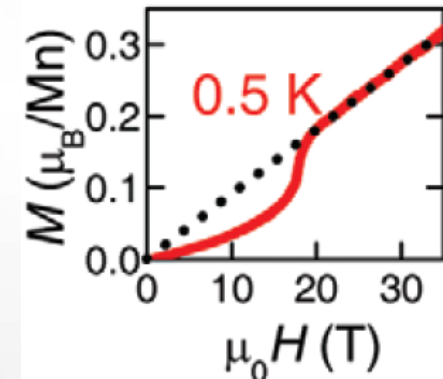
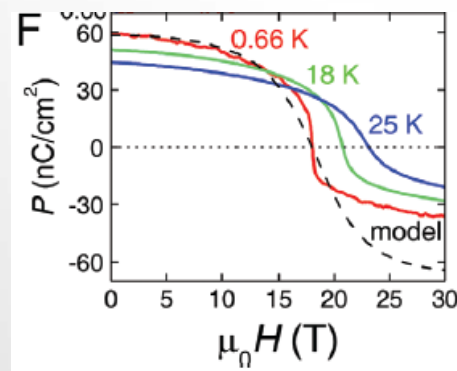


$$\mathcal{M} \equiv \frac{1}{6L_xL_y} \sum_i \sum_{\alpha=1}^6 \mathbf{S}_{i\alpha} \cdot \hat{x},$$

$$\mathcal{P} \equiv \frac{1}{L_xL_y} \frac{1}{J_3} \sum_i (u_i + d_i).$$

$T > T^*$  : continuous crossover

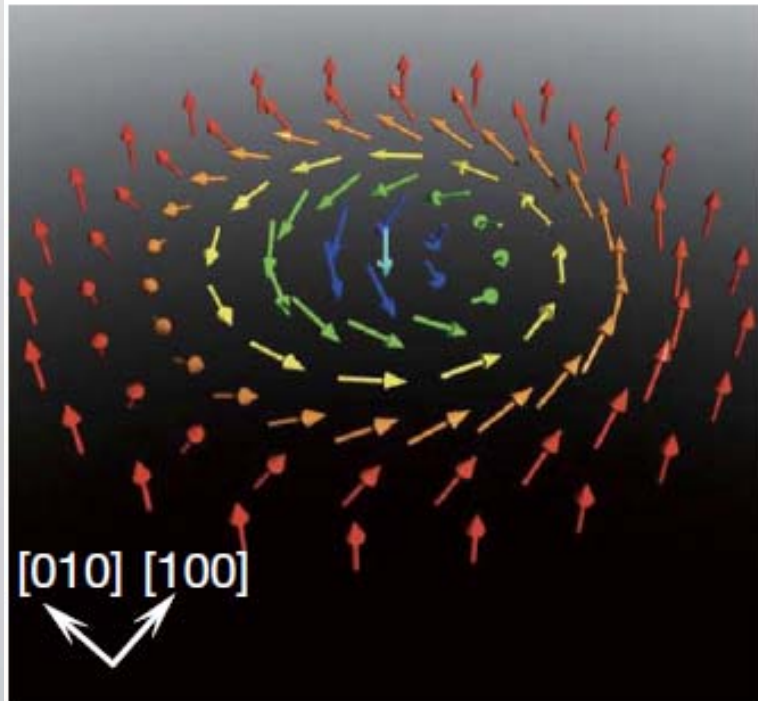
$T < T^*$  : first-order metaelectric transition





# Monte Carlo simulations: Skyrmion Crystal

# Skyrmion

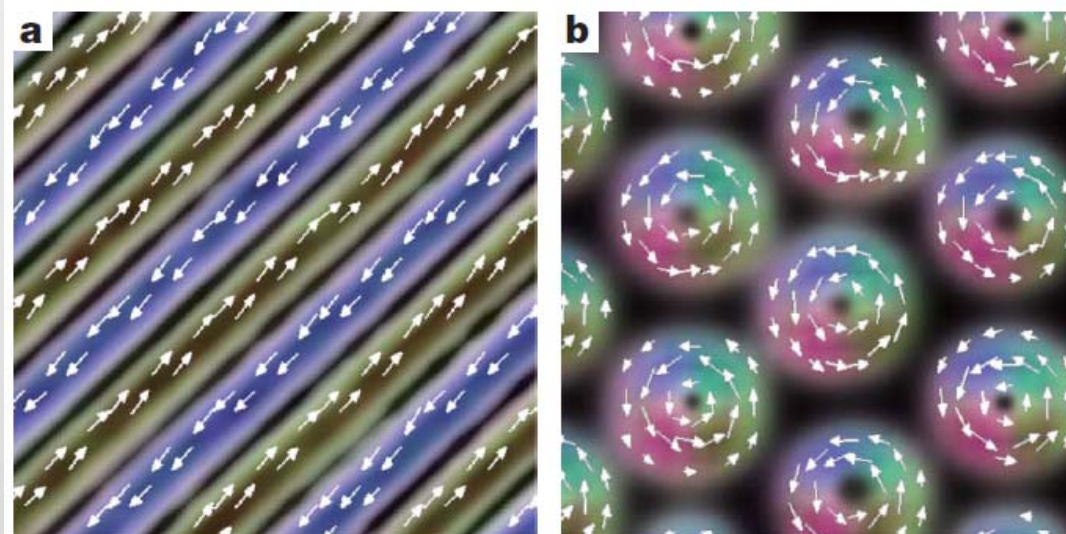


- Topological excitation in two-dimensional Heisenberg spin model
- Indirect NMR observation of skyrmions in two-dimensional quantum Hall ferromagnetic state

# Skyrmion Crystal

Monte Carlo simulations of the Hamiltonian

$$H = \int d\mathbf{r} \left[ \frac{J}{2} (\nabla \mathbf{M})^2 + \alpha \mathbf{M} \cdot (\nabla \times \mathbf{M}) \right]$$

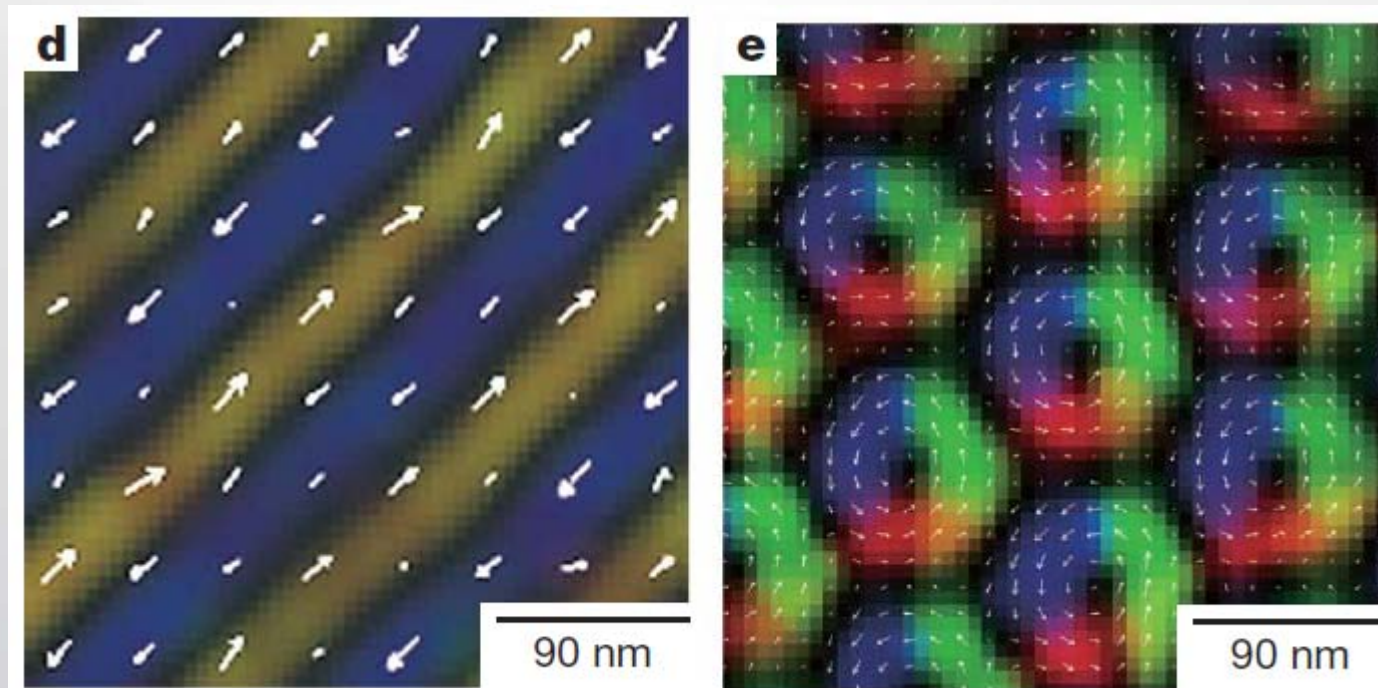


zero magnetic field

weak magnetic field

# Real-space observation of Skyrmion Crystal

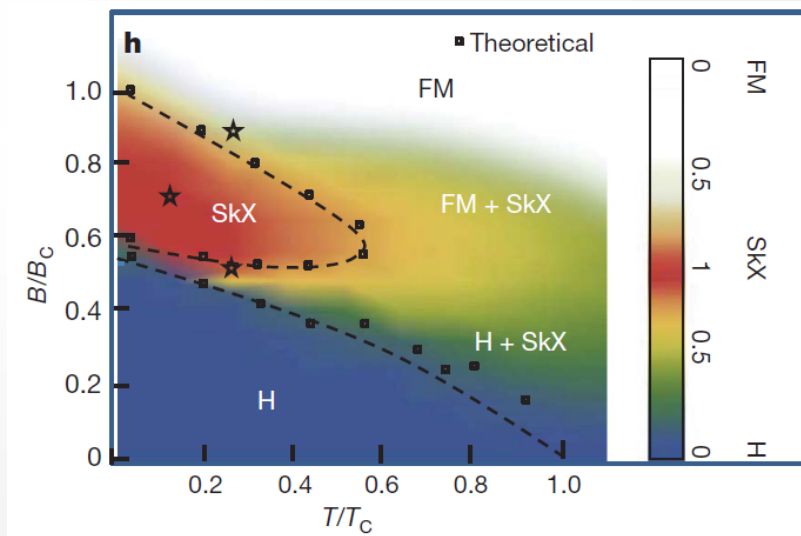
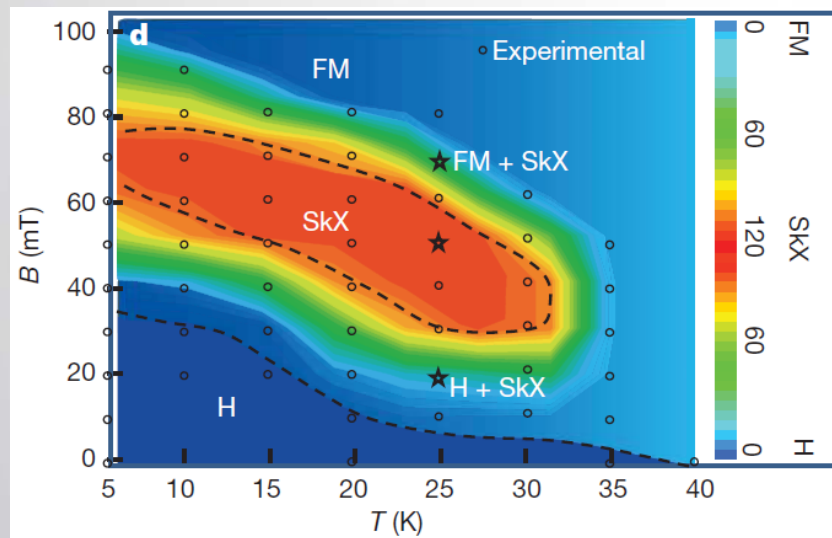
spin textures in the helical magnet  $\text{Fe}_{0.5}\text{Co}_{0.5}\text{Si}$




zero magnetic field

weak magnetic field

# Phase Diagram





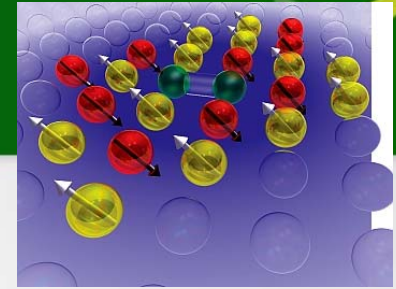
# Numerical Calculations in Quantum Theory of Many Particles

Example: Dynamical Mean-Field Theory

# Numerical Methods in Quantum Theory of Many Particles

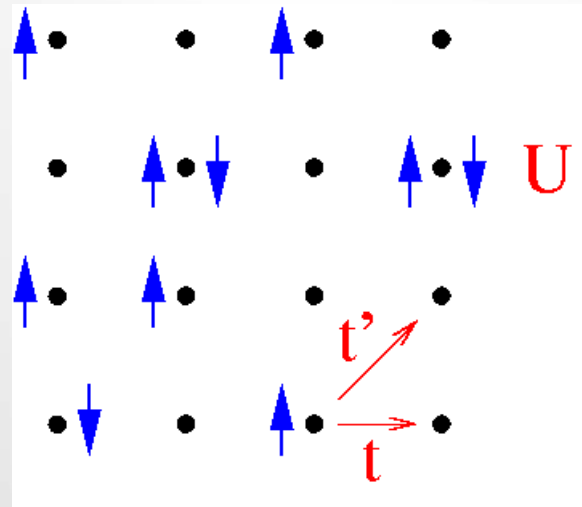
- Quantum Monte Carlo Method
- Density Matrix Renormalization Group
- Numerical Renormalization Group
- Exact Diagonalization
- Slave-Boson Theory
- Hartree-Fock Approximation
- Decoupling Method
- Dynamical Mean-Field Theory
- ...

# Hubbard model



$$H = - \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

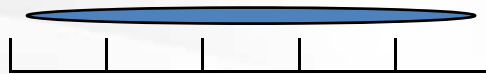
Tight-binding electrons with on-site Coulomb repulsion  $U$



# Mott-Hubbard Transition

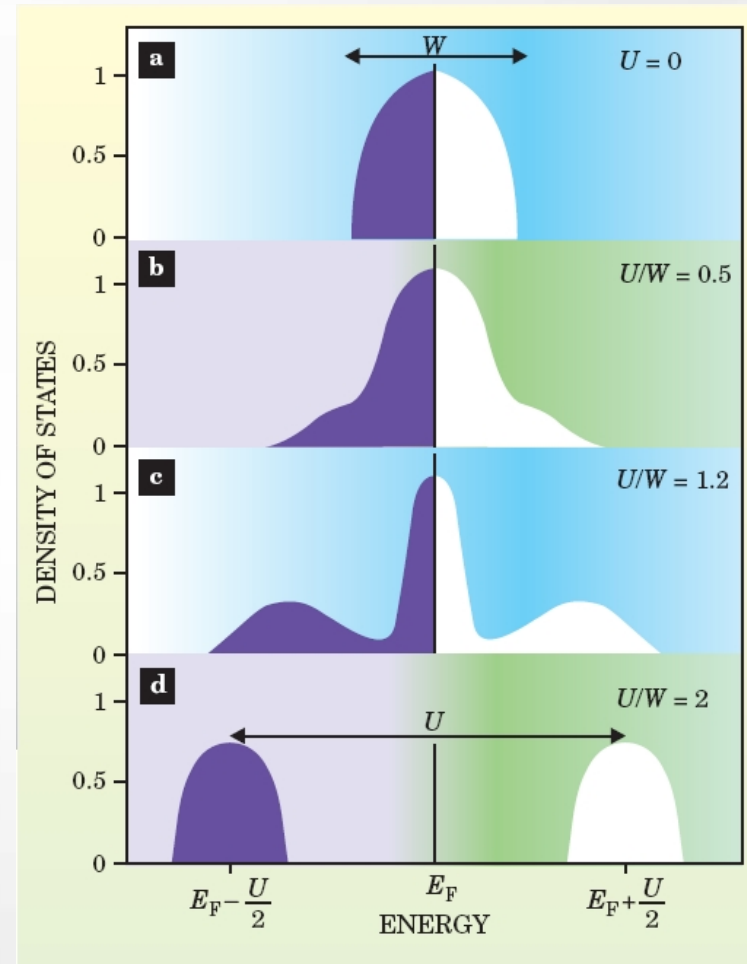
$$H = - \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Weakly  
correlated

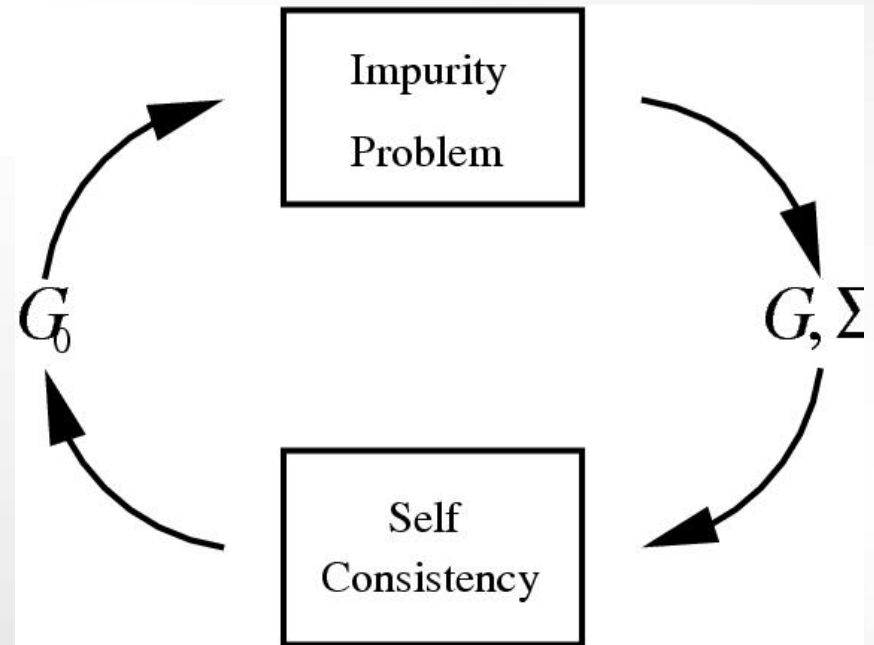
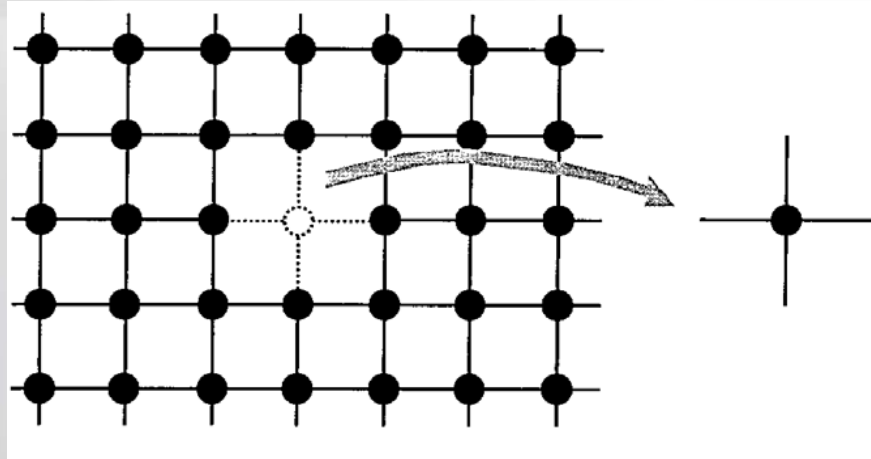


Intermediate regime :  
hard to describe quantitatively

Strongly  
correlated



# Dynamical Mean-Field Theory



# Weiss Mean-Field Theory: classical Ising model

$$H = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j - h \sum_i S_i$$

STEP 1: Construct an effective single-site model

$$\begin{aligned} H_{\text{eff}} &= -h_{\text{eff}} S_o \\ h_{\text{eff}} &= h + \sum_i J_{oi} \langle S_i \rangle = h + zJm \\ m &= \langle S_i \rangle, z: \text{coordination number} \end{aligned}$$

STEP 2: Solve a single-site model

$$\langle S_o \rangle = \tanh(\beta h_{\text{eff}})$$

STEP 3: Impose a self-consistent condition

$$\langle S_o \rangle = m$$

$$h_{\text{eff}} = h + zJ \langle S_o \rangle$$

# Weiss Mean-Field Theory: classical Ising model

$$H = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j - h \sum_i S_i$$

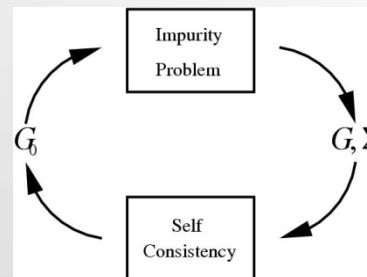
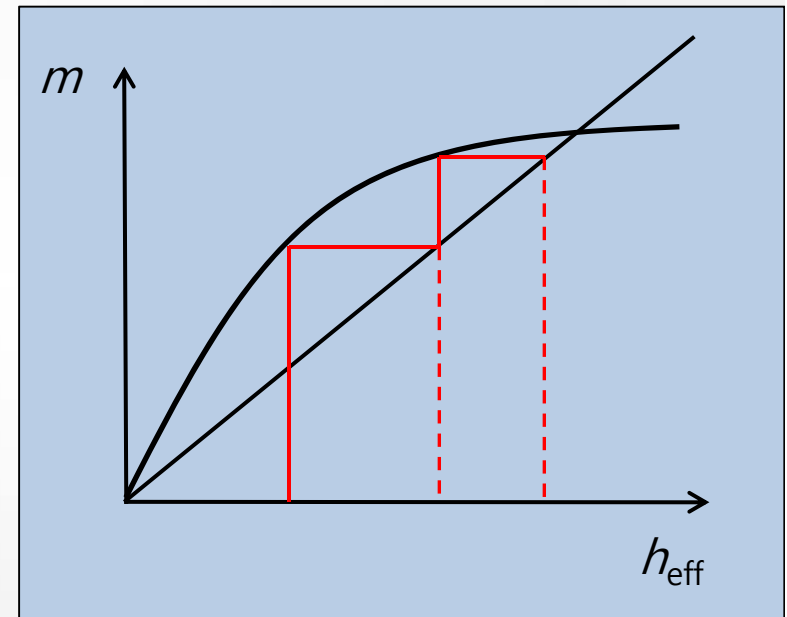
Weiss mean-field equation

$$m = \tanh(zJm + h)$$

Or

$$m = \tanh(\beta h_{\text{eff}})$$

$$h_{\text{eff}} = h + zJm : \text{Weiss field}$$



# Dynamical Mean-Field Theory Hubbard model

$$H = - \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

STEP 1: Construct an effective single-site (impurity) model

$$\begin{aligned} S_{\text{imp}} = & - \int_0^\beta d\tau \int_0^{\beta'} d\tau' \sum_\sigma c_{o\sigma}^\dagger(\tau) G_0^{-1}(\tau - \tau') c_{o\sigma}(\tau') \\ & + U \int_0^\beta d\tau n_{o\uparrow}(\tau) n_{o\downarrow}(\tau) \end{aligned}$$

$G_0(\tau - \tau')$ : Weiss field

creation/annihilation of electron at the site  
time-dependent

$$H_{\text{eff}} = -h_{\text{eff}} S_o$$

# Dynamical Mean-Field Theory Hubbard model

STEP 2: Solve a single-site (impurity) model

$$S_{\text{imp}} = - \int_0^\beta d\tau \int_0^{\beta'} d\tau' \sum_{\sigma} c_{o\sigma}^\dagger(\tau) G_0^{-1}(\tau - \tau') c_{o\sigma}(\tau') \\ + U \int_0^\beta d\tau n_{o\uparrow}(\tau) n_{o\downarrow}(\tau)$$

impurity Green function

$$G_{\text{imp},\sigma}(\tau - \tau') = - \langle T c_{o\sigma}(\tau) c_{o\sigma}^\dagger(\tau') \rangle_{S_{\text{imp}}}$$

impurity self-energy

$$\Sigma_{\text{imp}} = G_{\text{imp}}^{-1} - G_0^{-1}$$

$$\langle S_o \rangle = \tanh(\beta h_{\text{eff}})$$

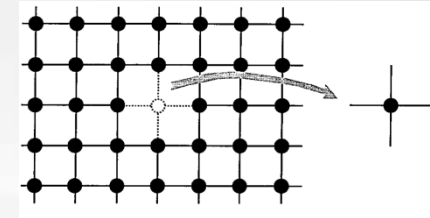
# Dynamical Mean-Field Theory Hubbard model

STEP 3: Impose a self-consistent condition

$$\begin{aligned} G_{\text{imp}}(\omega) &= G_{\text{loc}}(\omega) \\ &= \sum_{\mathbf{k}} \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\text{imp}}(\omega)} \end{aligned}$$

$$\Sigma_{\text{imp}} = \text{ImpuritySolver}[G_0, U]$$

$$G_0^{-1} = G_{\text{loc}}[\Sigma_{\text{imp}}]^{-1} - \Sigma_{\text{imp}}$$



$$\langle S_o \rangle = m$$

$$m = \tanh(\beta h_{\text{eff}})$$

$$h_{\text{eff}} = h + zJm : \forall$$

# Mean-Field Theory

## Classical vs. Quantum

$$H = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j - h \sum_i S_i$$

$$H = - \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$m = \langle S_i \rangle$$

$$G_{ii}(\omega) \quad \text{or} \quad \Sigma_{ii}(\omega)$$

$$h_{\text{eff}} = zJm + h$$

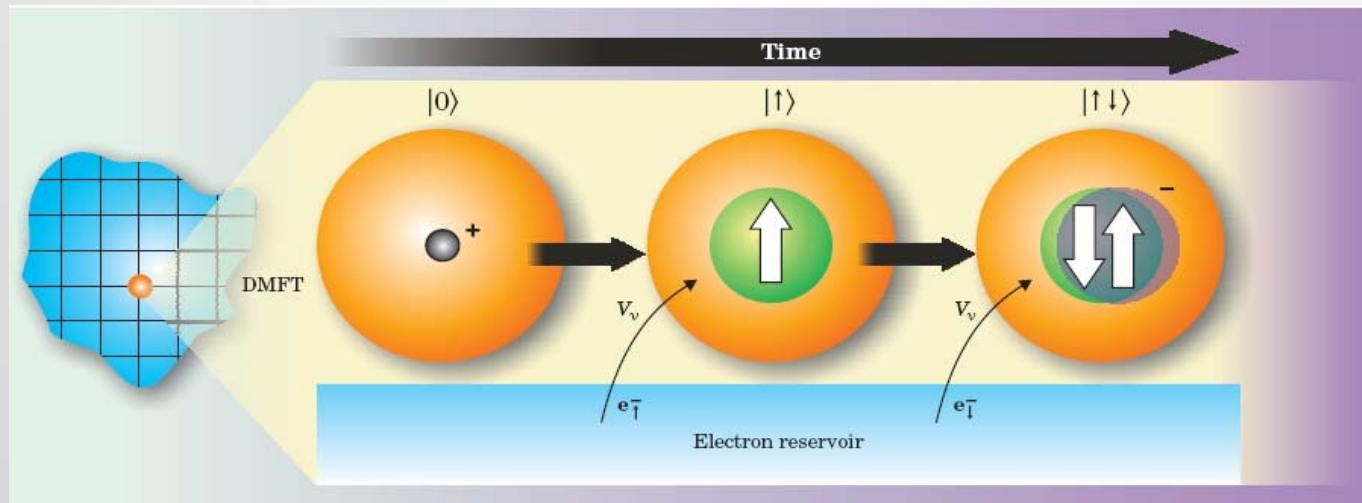
$$G_0(\omega)$$

$$m = \tanh(\beta h_{\text{eff}})$$

$$\Sigma_{\text{imp}} = \text{ImpuritySolver}[G_0, U]$$

# Why DMFT?

- ❖ Non-perturbative and time-resolved treatment of local interactions
- ❖ Unified description of metals and Mott insulators



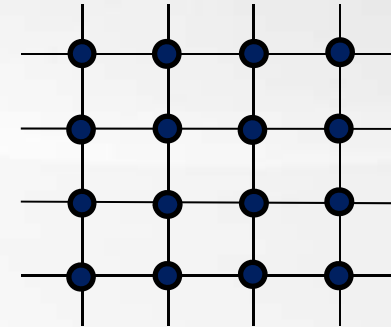
# How to Solve Impurity Problem

- Exact Diagonalization (ED)
- Quantum Monte Carlo (QMC)
  - continuous time QMC
  - Hirsch-Fye QMC
  - Projective QMC
- Numerical renormalization group
- Density matrix renormalization group
  
- Non-Crossing Approximation
- Iterated Perturbation Theory
- Hubbard Approximations
- ...

# DMFT + ED

- ◇ Lattice problem (ex. Hubbard model)

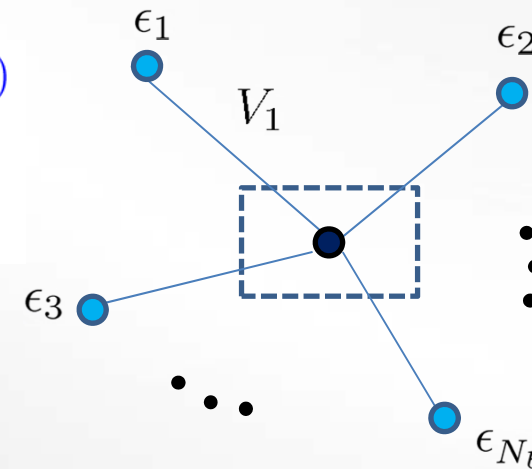
$$H = -t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}$$



- ◇ Impurity problem

$$H_{\text{imp}} = \sum_{l\sigma} \epsilon_{l\sigma} a_{l\sigma}^\dagger a_{l\sigma} + \sum_{l\sigma} V_{l\sigma} (a_{l\sigma}^\dagger c_{o\sigma} + c_{o\sigma}^\dagger a_{l\sigma}) - \mu \sum_{\sigma} c_{o\sigma}^\dagger c_{o\sigma} + U n_{o\uparrow} n_{o\downarrow}$$

+ Self-consistent equations for bath parameters



# DMFT + ED (1)

$$\Sigma_{\text{imp}} = \text{ImpuritySolver}[G_0, U]$$

$$G_0^{-1} = G_{\text{loc}}[\Sigma_{\text{imp}}]^{-1} - \Sigma_{\text{imp}}$$

$$\mathcal{G}_0(i\omega_n)^{-1} = i\omega_n + \mu - \int_{-\infty}^{+\infty} d\omega' \frac{\Delta(\omega')}{i\omega_n - \omega'}$$

$$\mathcal{G}_0^{n_s}(i\omega_n)^{-1} = i\omega_n + \mu - \sum_{p=2}^{n_s} \frac{V_p^2}{i\omega_n - \tilde{\epsilon}_p}$$

- Prepare initial sets of  $\{ V_p, \epsilon_p \}$

# DMFT + ED (2)

$$\Sigma_{\text{imp}} = \text{ImpuritySolver}[G_0, U]$$

$$G_0^{-1} = G_{\text{loc}}[\Sigma_{\text{imp}}]^{-1} - \Sigma_{\text{imp}}$$

$$G(i\omega_n) = \frac{1}{Z} \sum_{i,j} \frac{(\langle i|d^+|j\rangle)^2}{E_i - E_j - i\omega_n} \times [\exp(-\beta E_i) + \exp(-\beta E_j)].$$

Lanczos method

$$G^>(\omega) = \frac{\langle \text{g.s.} | dd^\dagger | \text{g.s.} \rangle}{\omega - a_0^> - \frac{b_1^{>2}}{\omega - a_1^> - \frac{b_2^{>2}}{\omega - a_2^> - \dots}}},$$
$$G^<(\omega) = \frac{\langle \text{g.s.} | d^\dagger d | \text{g.s.} \rangle}{\omega - a_0^< - \frac{b_1^{<2}}{\omega - a_1^< - \frac{b_2^{<2}}{\omega - a_2^< - \dots}}}.$$

# DMFT + ED (3)

$$\Sigma_{\text{imp}} = \text{ImpuritySolver}[G_0, U]$$

$$G_0^{-1} = G_{\text{loc}}[\Sigma_{\text{imp}}]^{-1} - \Sigma_{\text{imp}}$$

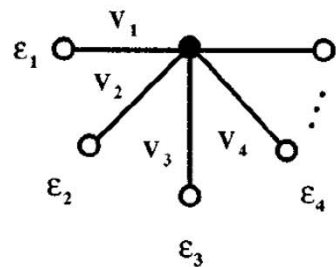
$$\mathcal{G}_0^{n_s}(i\omega_n)^{-1} = i\omega_n + \mu - \sum_{p=2}^{n_s} \frac{V_p^2}{i\omega_n - \tilde{\epsilon}_p}$$

$$d = \frac{1}{n_{\text{max}} + 1} \sum_{n=0}^{n_{\text{max}}} |\mathcal{G}_0(i\omega_n)^{-1} - \mathcal{G}_0^{n_s}(i\omega_n)^{-1}|^2$$

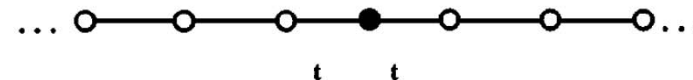
Minimize  $d$  to yield new sets of  $\{ V_p, \epsilon_p \}$

# Bath Geometry (DMFT+ED)

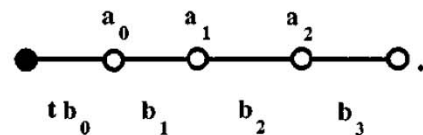
Star



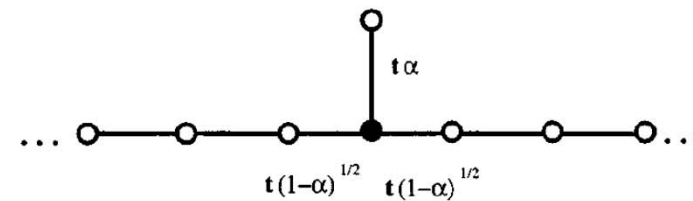
Two Chain



Chain



Mixed



# DMFT + CTQMC

## Continuous-Time Quantum Monte Carlo method (CT-QMC)

- general formalism

1. model Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

2. partition function expansion in interaction picture

$$\begin{aligned} Z &= \text{tr} \left[ e^{-\beta \mathcal{H}} \right] \\ &= \sum_k (-1)^k \int_{\tau_{k-1}}^{\beta} d\tau_k \cdots \int_0^{\beta} d\tau_1 \text{tr} \left[ e^{-\beta \mathcal{H}_0} \hat{\mathcal{H}}_1(\tau_k) \cdots \hat{\mathcal{H}}_1(\tau_1) \right] \end{aligned}$$

3. partition function as an integral over configuration  $\mathbf{x} \in \mathcal{C}$  with weight  $p(\mathbf{x})$ .

$$Z = \int_{\mathcal{C}} d\mathbf{x} p(\mathbf{x})$$

4. stochastic sampling of observables
  - Green's function

by AJK

# DMFT + CTQMC

- weak coupling algorithm (CT-AUX)

1. expansion term

$$\mathcal{H}_1 = U \left( n_\uparrow n_\downarrow - \frac{n_\uparrow + n_\downarrow}{2} \right)$$

2. Hubbard-Stratonovich transform

$$1 - \frac{\beta U}{K} \left( n_\uparrow n_\downarrow - \frac{n_\uparrow + n_\downarrow}{2} \right) = \frac{1}{2} \sum_{s=\pm 1} e^{\gamma s (n_\uparrow - n_\downarrow)}$$

3. configuration space with auxiliary Ising fields

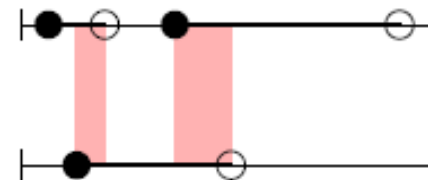


- strong coupling algorithm (CT-HYB)

1. expansion term

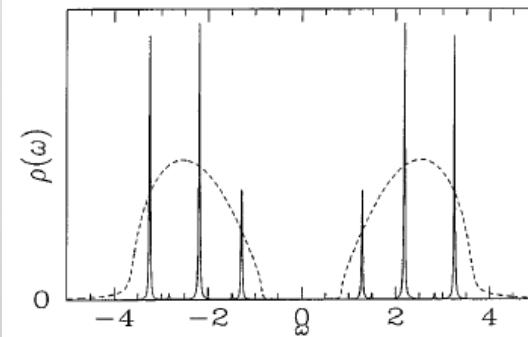
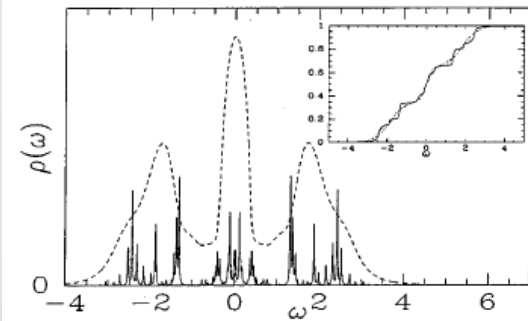
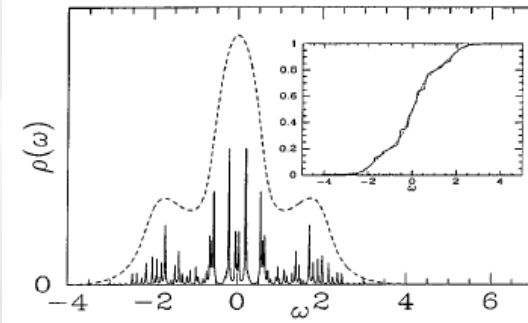
$$\mathcal{H}_1 = \sum_{\sigma,p} (V_p^\sigma d_\sigma^\dagger a_{p,\sigma} + h.c.)$$

2. configuration space with segments for density-density interaction



by AJK

# DMFT+ED (IPT)



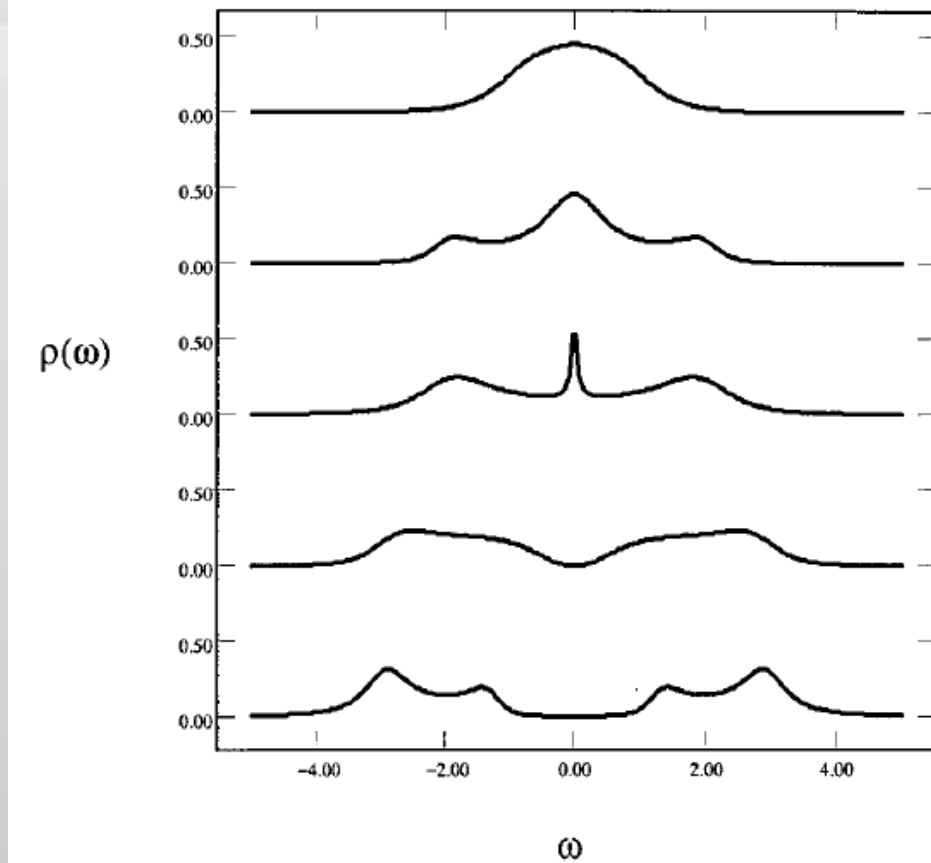
Metal

U

Insulator

*Caffarel, Krauth (1994)*  
*Georges, Kotliar, Krauth, Rozenberg (1996)*

# DMFT+QMC (Hirsch-Fye)



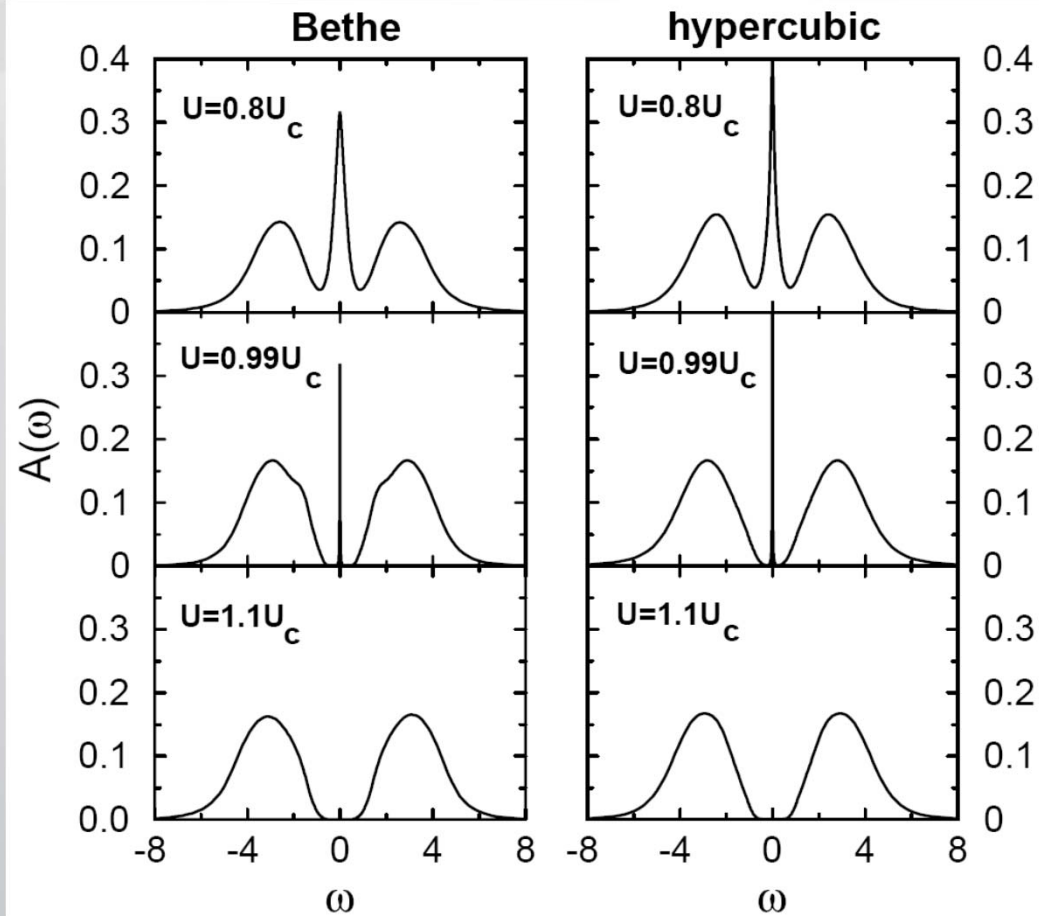
Metal

$U$

Insulator

*Georges, Kotliar, Krauth, Rozenberg (1996)*

# DMFT + NRG

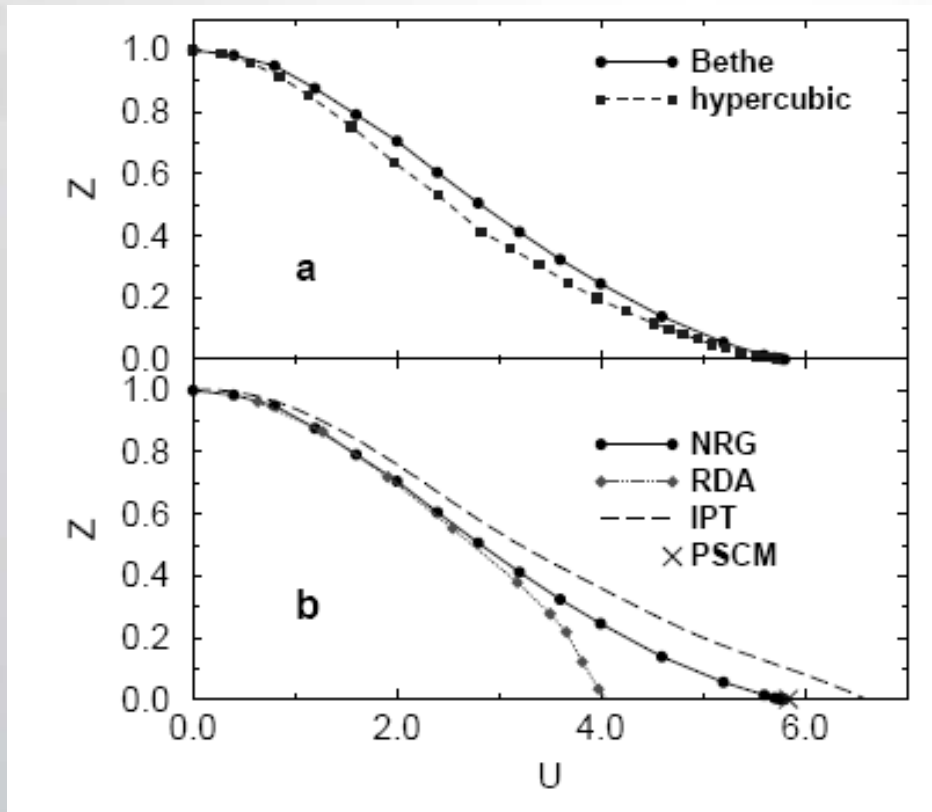


Metal-insulator transition at

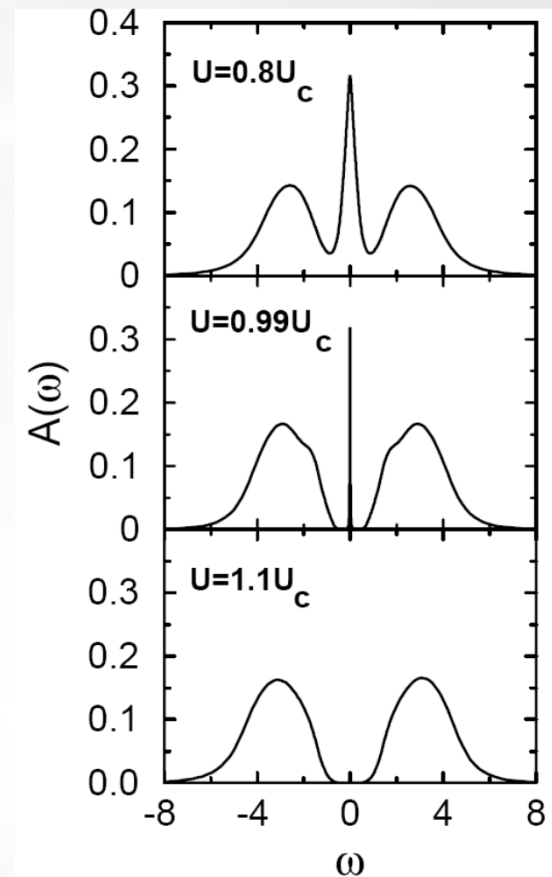
- $U_{c2} = 1.47W$
- $U_{c1} = 1.25W$

*Bulla, PRL (1999)*

# Quasiparticle weight (DMFT+NRG)



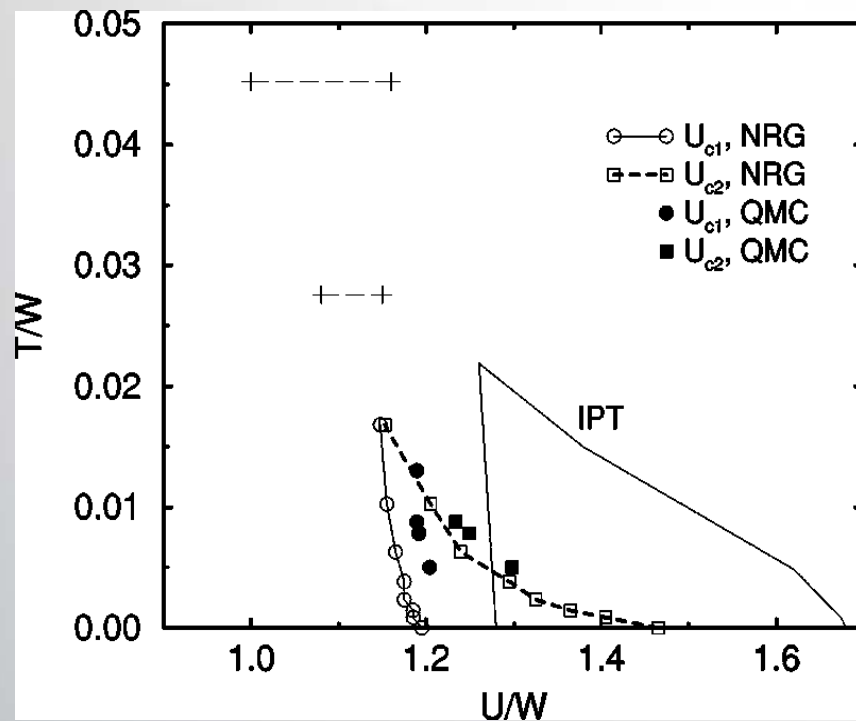
$$Z = \frac{1}{1 - \left. \frac{\partial \Re e \Sigma(\omega)}{\partial \omega} \right|_{\omega=0}},$$



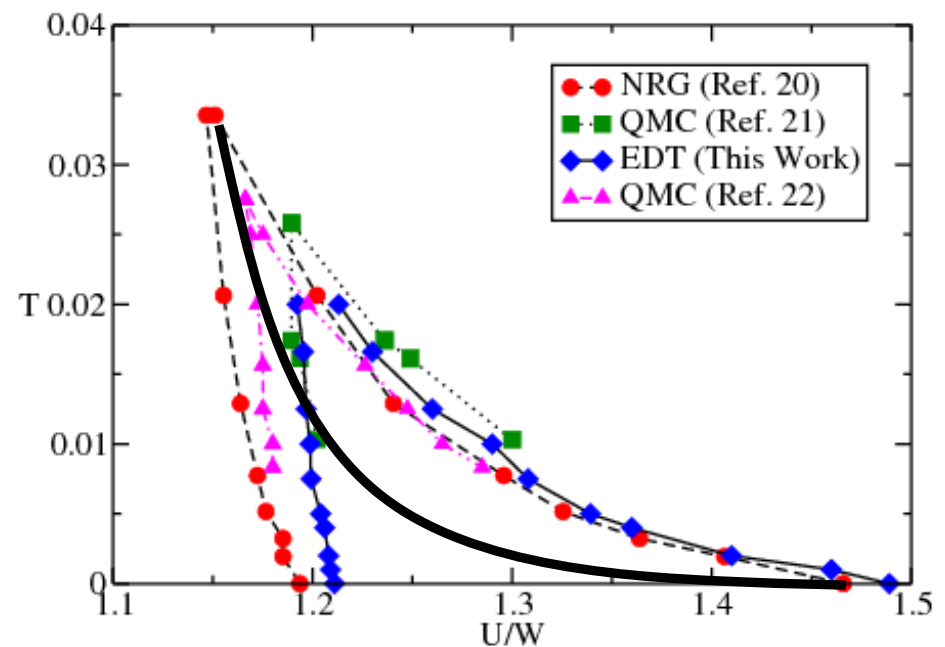
*Bulla, PRL (1999)*

# Phase Diagram

- Existence of coexistence region
- First-order transition line ends at finite-temperature critical point
- Crossover region above a critical point

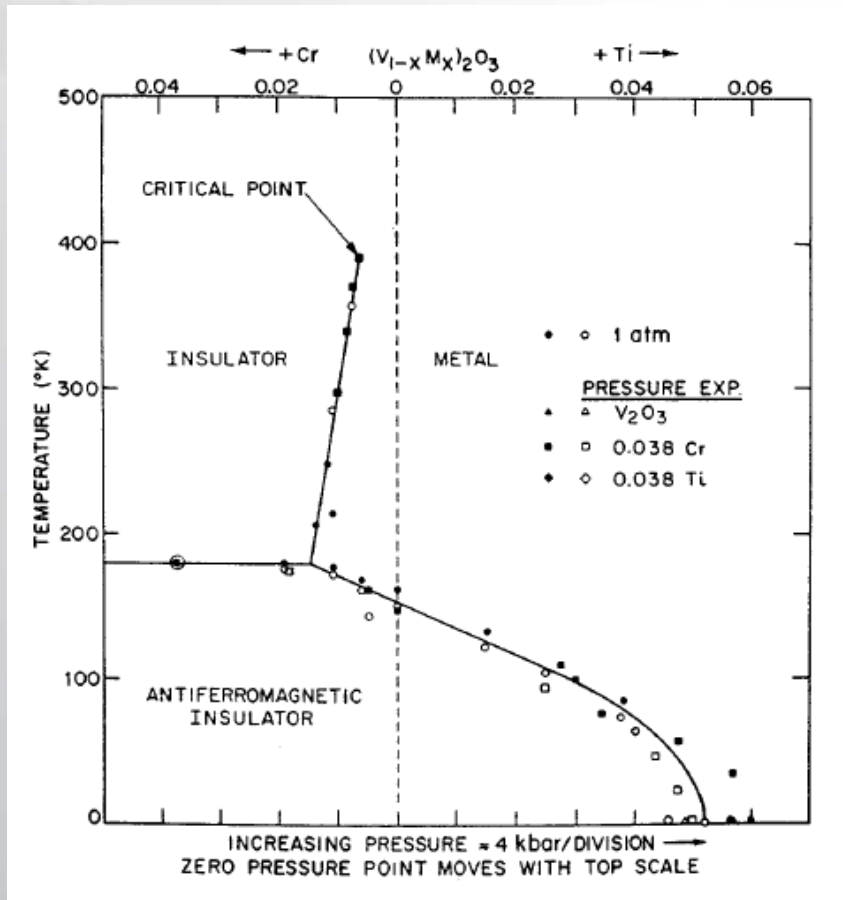


*Bulla, Costi, Vollhardt, PRB(2001)*

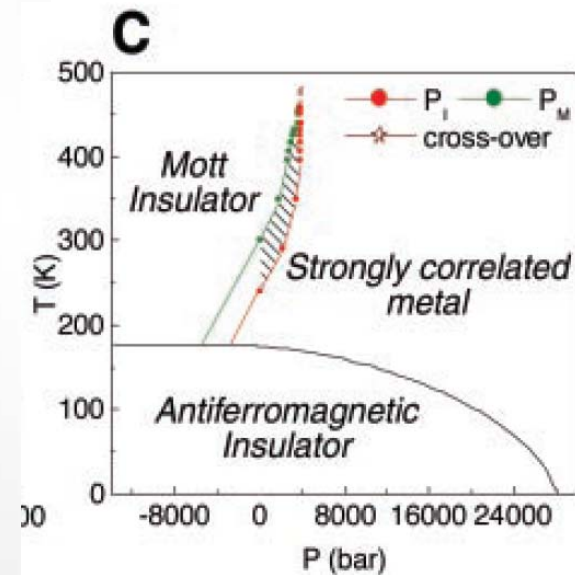
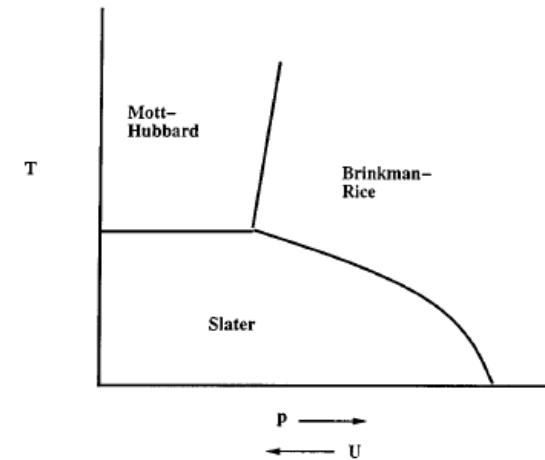


*Capone, Medici, Georges (2007)*

# Phase Diagram of $V_2O_3$

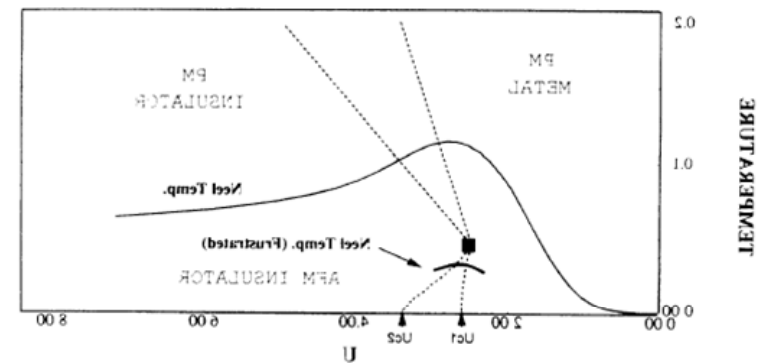
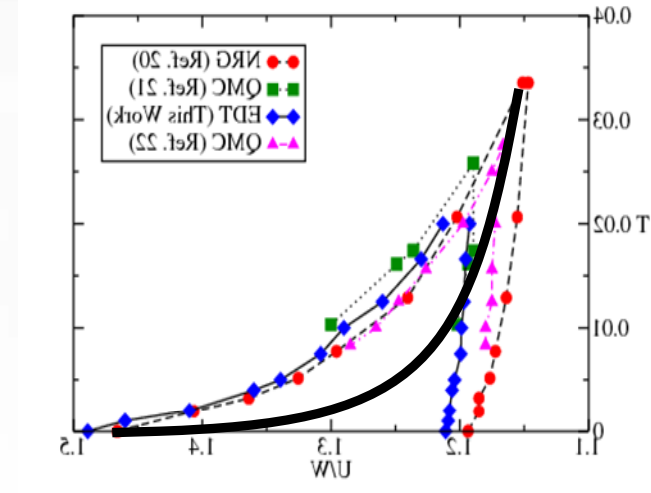
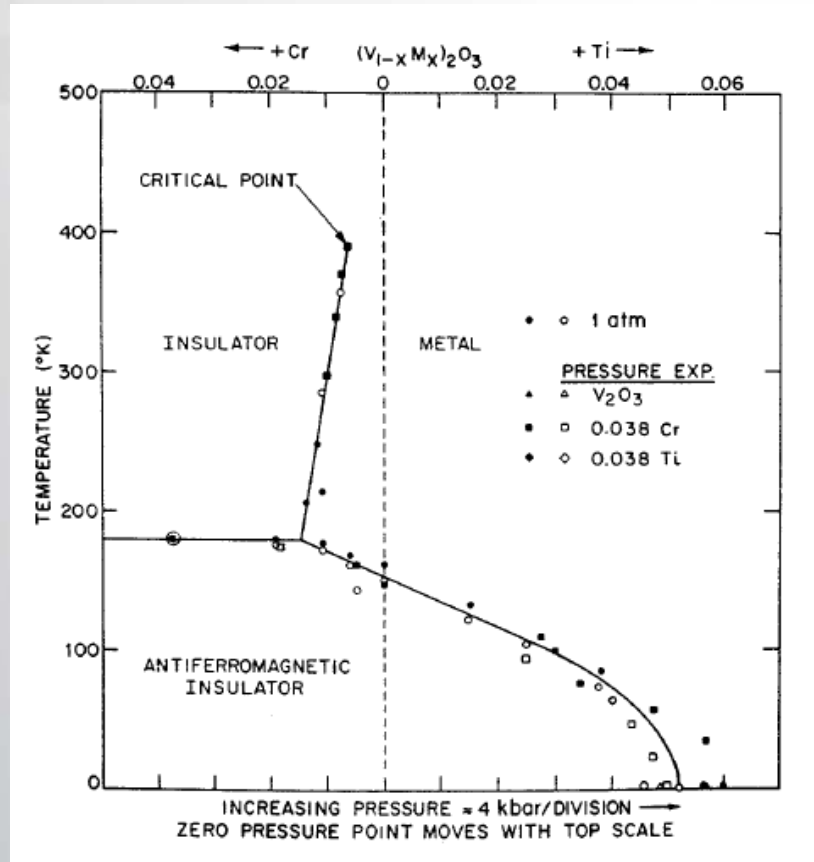


McWhan et al. PRL (1971)



Limelette, Georges, Jerome, Wzietek, Metcal f, Honig, Science (2003)

# Phase Diagram of $V_2O_3$



**DMFT** : first unified framework for various phases

# Concluding Remark

Let's play with computers.

Let's play with condensed matter physics.