Magnetic models and phase transitions

Phase transitions

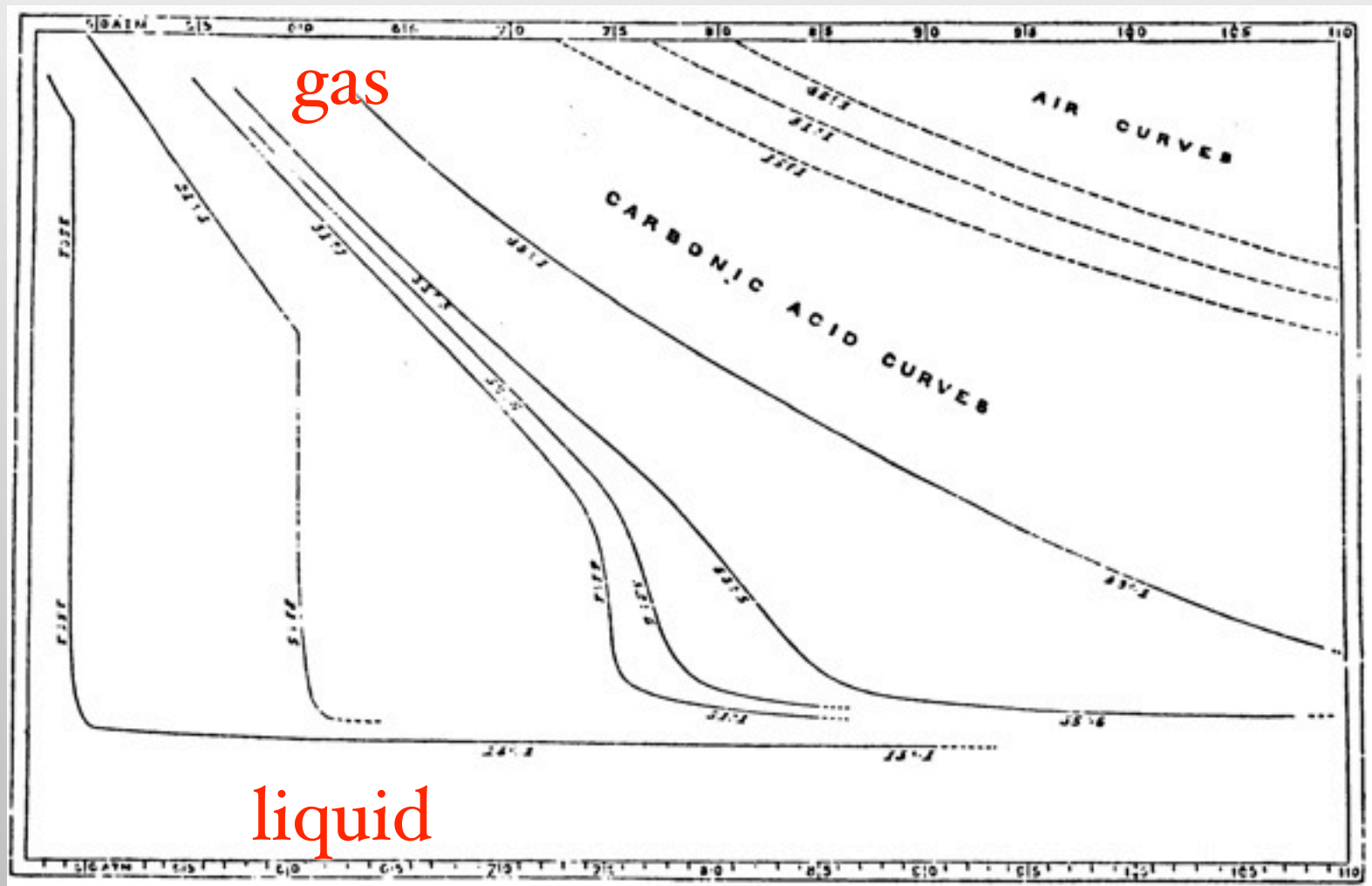
Are a central topic of statistical physics

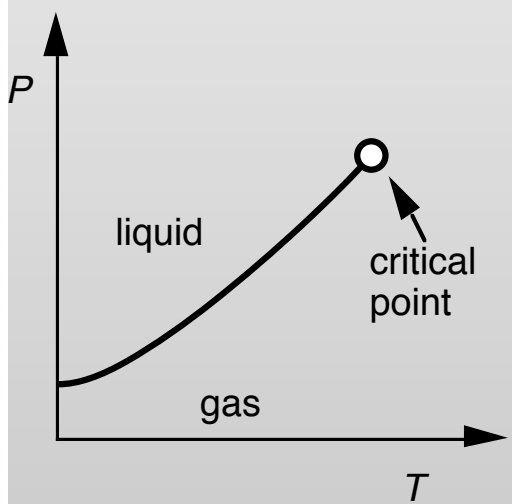
Increasing temperature

solid liquid gas

1869: Andrew's Talk at the Royal Society

- Critical point of the liquid-gas transition in CO_2
  - Below T_c=30.92 °C: clear distinction between liquid and gas
  - Above T_c: no distinction



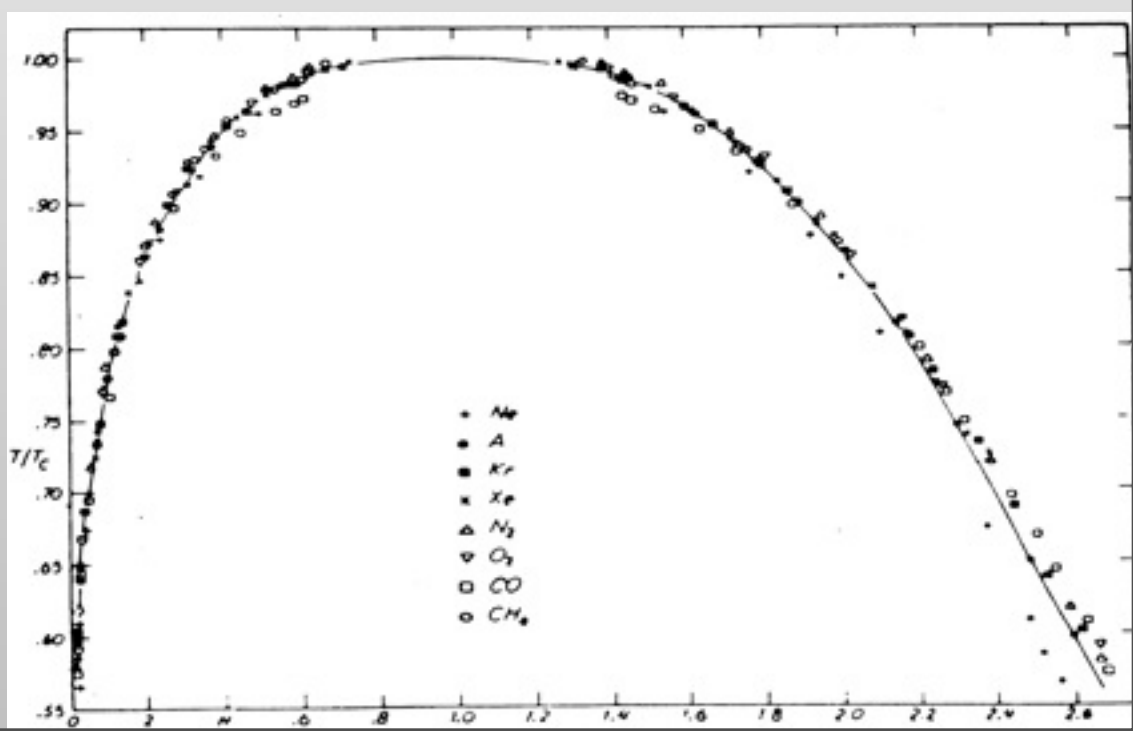


1874 van der Waals and Maxwell

- Van der Waals equation

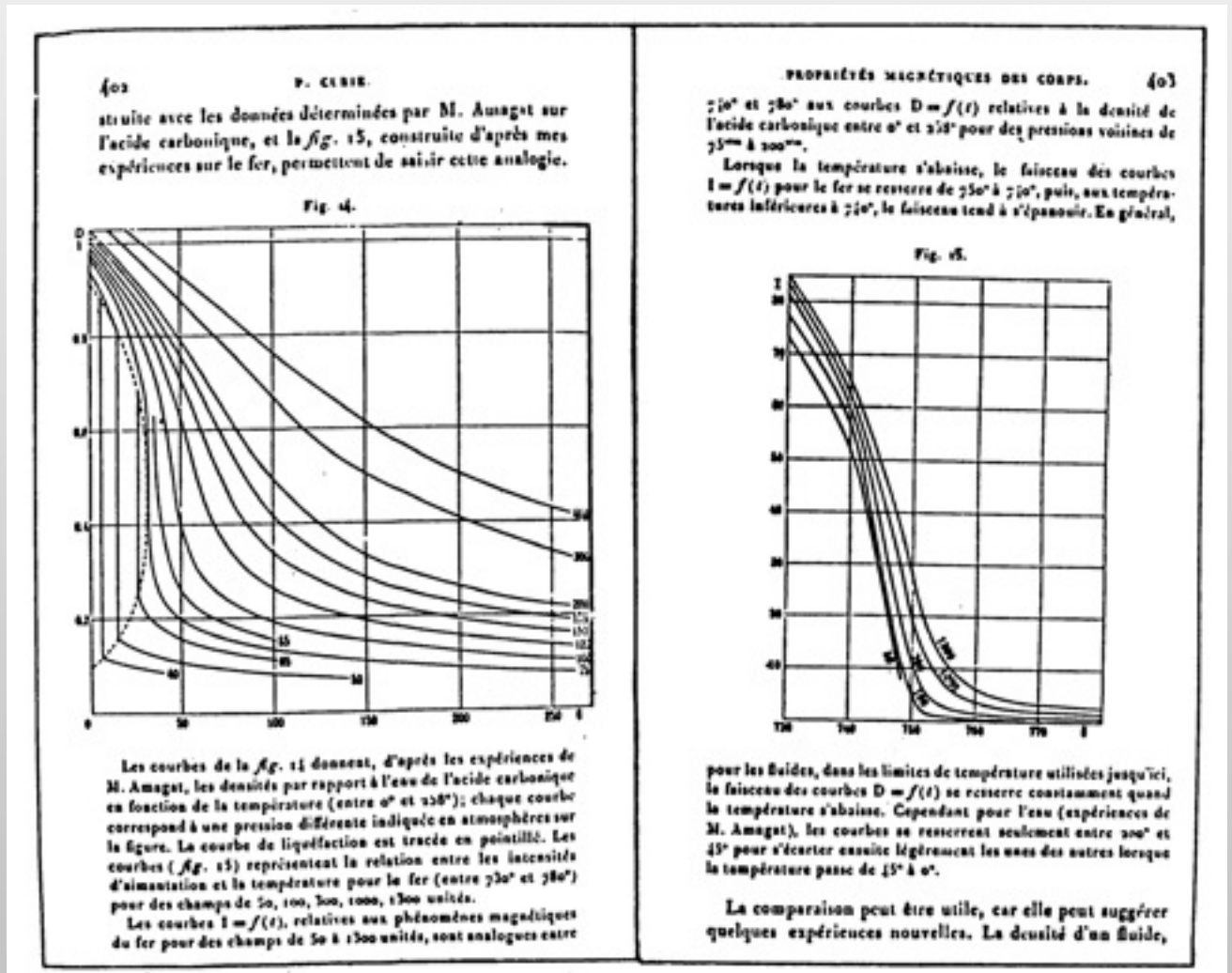
$$(P + a/v^2)(v - b) = RT$$

  - Three solutions $T < T_c$ (gas, liquid and unphysical)
  - Maxwell-construction explains coexistence of gas and liquid
- Universal behavior in reduced dimensions (T/T_c, ρ/ρ_c, p/p_c, ...)
  - Expermimentally verified
  - But cubic instead of quadratic behavior (van der Waals)



1895: Pierrre Curie

- Magnetism is similar to liquids
- Magnetic susceptibility diverges (Curie law)



402 P. CURIE.

struite avec les données déterminées par M. Amagat sur l'acide carbonique, et la *fig.* 15, construite d'après mes expériences sur le fer, permettent de saisir cette analogie.

Fig. 14.

Les courbes de la *fig.* 14 donnent, d'après les expériences de M. Amagat, les densités par rapport à l'eau de l'acide carbonique en fonction de la température (entre 0° et 258°); chaque courbe correspond à une pression différente indiquée en atmosphères sur la figure. La courbe de liquéfaction est tracée en pointillé. Les courbes (*fig.* 15) représentant la relation entre les intensités d'aimantation et la température pour le fer (entre 730° et 780°) pour des champs de 50, 100, 300, 1000, 1300 unités.

Les courbes $I = f(t)$, relatives aux phénomènes magnétiques du fer pour des champs de 50 à 1300 unités, sont analogues entre

PROPRIÉTÉS MAGNÉTIQUES DES CORPS. 403

730° et 780° aux courbes $D = f(t)$ relatives à la densité de l'acide carbonique entre 0° et 258° pour des pressions voisines de 75^{atm} à 200^{atm}.

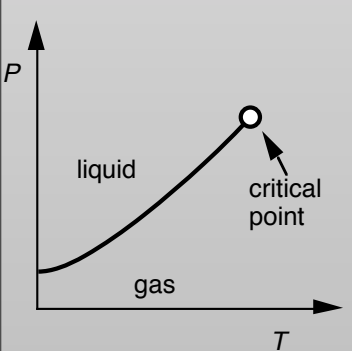
Lorsque la température s'abaisse, le faisceau des courbes $I = f(t)$ pour le fer se resserre de 750° à 730°, puis, aux températures inférieures à 730°, le faisceau tend à s'épanouir. En général,

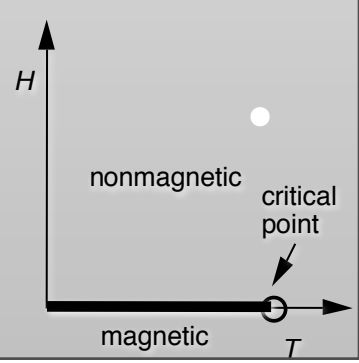
Fig. 15.

pour les fluides, dans les limites de température utilisées jusqu'ici, le faisceau des courbes $D = f(t)$ se resserre constamment quand la température s'abaisse. Cependant pour l'eau (expériences de M. Amagat), les courbes se resserrent seulement entre 200° et 45° pour s'écarter ensuite légèrement les unes des autres lorsque la température passe de 45° à 0°.

La comparaison peut être utile, car elle peut suggérer quelques expériences nouvelles. La densité d'un fluide,

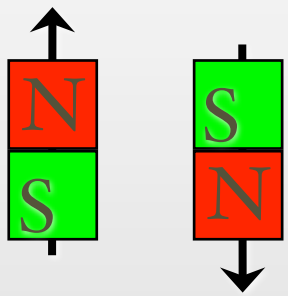
$$\chi = \frac{C}{T - T_C}$$





The Ising model

- Ising model
  - molecular magnets with two states
  - north pole up or down



- Magnetic moments prefer to align
  - parallel: energy -J ↑↑ or ↓↓
  - anti-parallel: energy +J ↑↓ or ↓↑

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

- Phase transition:
  - low temperatures: magnetically ordered

↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑

  - high temperatures : disordered

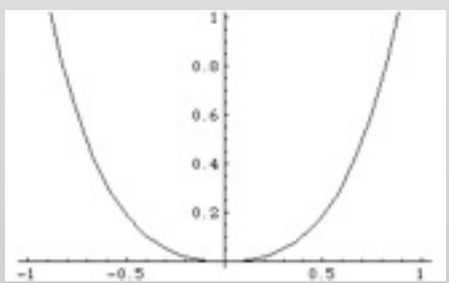
↑↓↓↑↓↑↑↓↓↓↑↑↓↑↓↓↑↑↓↑↓↓

1937: L.D. Landau

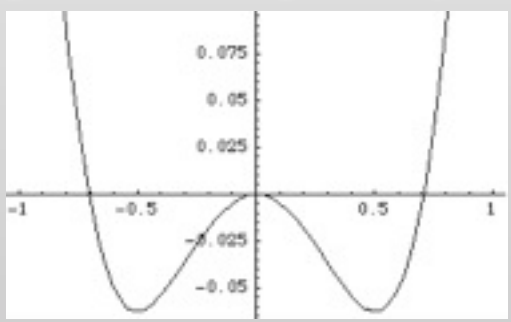
- Landau-Theory of phase transitions
  - Power series expansion of free energy:

$$F(P,T,\eta) = F_0(P,T) + A(P,T)\eta^2 + B(P,T)\eta^4 + \ldots$$

T > Tc: A > o
Minimum at η = o
Nonmagnetic



T < Tc: A < o
Two minima at $\eta = \pm\sqrt{-A/2B}$
magnetic, or gas/liquid



Divergences at critical point: T = Tc, A= o

$$M \propto (T_c - T)^{1/2} \qquad \chi \propto |T - T_c|^{-1}$$

1944/49: Onsager 1971: Wilson

- Landau-Theory explain everything! Are we done?
- 1944: Onsager solves Ising model exactly in two dimensions
  - Landau-Theory $M \propto (T_c - T)^{1/2}$
  - Onsager's solution $M \propto (T_c - T)^{1/8}$
- What is happening?
  - Landau-Theory predicts power laws
  - But the powers are not always right!
- 1971: Wilson's renormalization group theory
  - Explains existence of power laws
  - But cannot predict exponents: numerical simulations are needed

Magnetic phase transition

$T<T_c$

ferromagnet, $m>0$

Close to T_c:

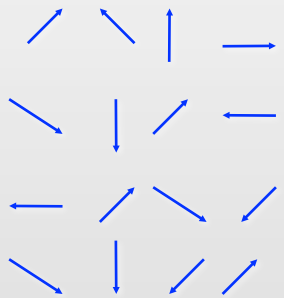
universal behavior

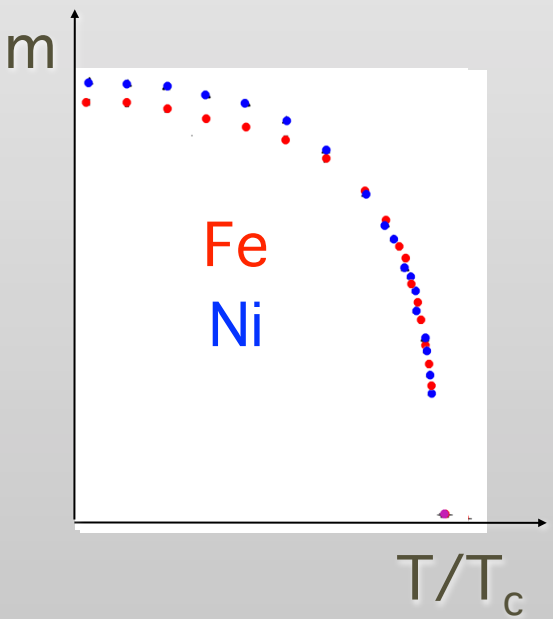
$$m \propto (T_c - T)^{\beta}$$

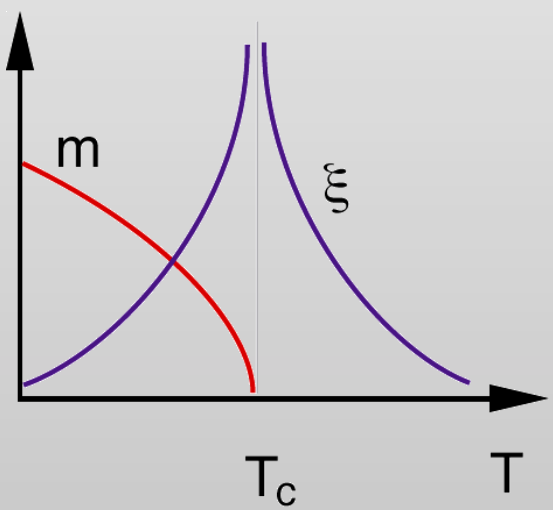
$$\xi \propto | T - T_c |^{-\nu}$$

$T>T_c$

Non-magnetic, $m = 0$







3D Heisenberg	β
Landau Mean-field	1 / 2
Monte Carlo	0.364(4)
Fe	0.34(4)
Ni	0.378(4)
$CrBr_3$	0.368(5)
Eu0	0.36(1)

numerical simulations essential to determine universal exponents β, ν

Critical behavior of magnetic models

$$M=\sum_i \sigma_i$$

Magnetization	$m=\langle \lvert M \rvert \rangle / V \propto (T_c - T)^{\beta}$
Susceptibility	$\chi=\dfrac{\langle M^2 \rangle - \langle \lvert M \rvert \rangle^2}{VT} \propto \lvert T_c - T \rvert^{-\gamma}$
Correlation function	$\langle \sigma_0 \sigma_{\mathbf{r}} \rangle - \langle \lvert m \rvert \rangle^2 \propto \exp(-r/\xi)$
Correlation length	$\xi \propto \lvert T_c - T \rvert^{-\nu}$
Correlation function at T_c	$\langle \sigma_0 \sigma_{\mathbf{r}} \rangle \propto r^{-(d-2+\eta)}$
Specific heat	$C = \dfrac{\partial E}{T} = \dfrac{\langle E^2 \rangle - \langle E \rangle^2}{T^2} \propto \lvert T_c - T \rvert^{-\alpha}$
Specific heat for 2D Ising model	$C \propto \ln \lvert T_c - T \rvert$

- **Values of critical exponents need to be calculated numerically**

Solving the Ising model

- We want to calculate a thermal average of some quantity A

$$\langle A \rangle = \sum_c A_c e^{-E_c/T} / Z \quad \text{with} \quad Z = \sum_c e^{-E_c/T}$$

- What is the complexity?
  - 2 states per spin
  - 2^N states for N spins: exact solution for at most 40 spins
- Exact solutions
  - One dimension: solution by transfer matrix method: phase transition at T_c=0
  - Square lattice: famous exact solution by Onsager
- What about higher dimensions, more complicated lattices or models?
- Mean field solution shown on blackboard
  - Is simple but gives wrong exponents

Numerical simulations

- "You let the computer solve the problem for you"

- It's not that easy:

  - Exponentially diverging number of states ✔
    - 1 site: q states
    - N sites: q^N states
  - Critical slowing down of the dynamics at phase transitions ✔
  - negative sign problem for fermions (NP-hard) ✗

GUEST EDITORS' INTRODUCTION

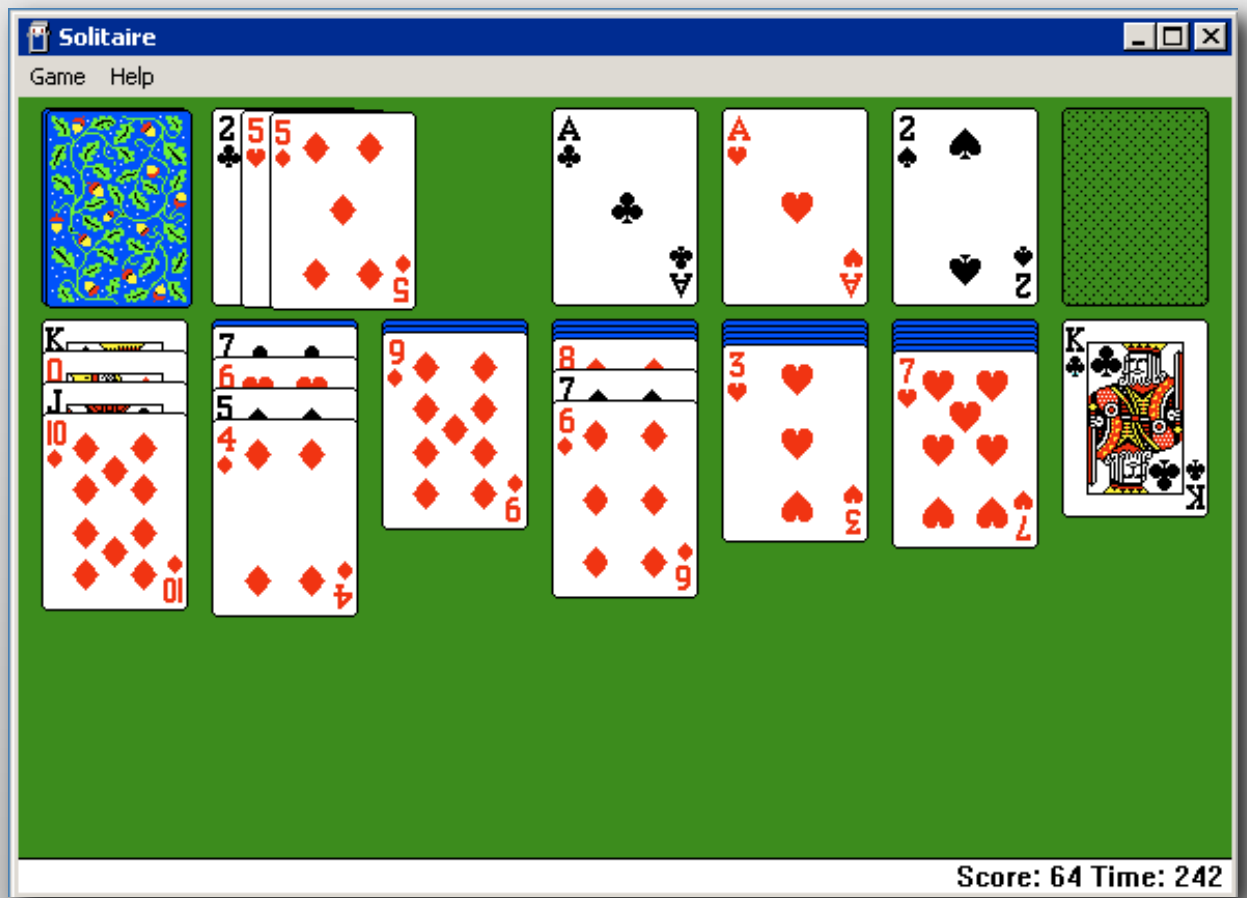
the Top 10 Algorithms

- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform
- Integer Relation Detection
- Fast Multipole Method

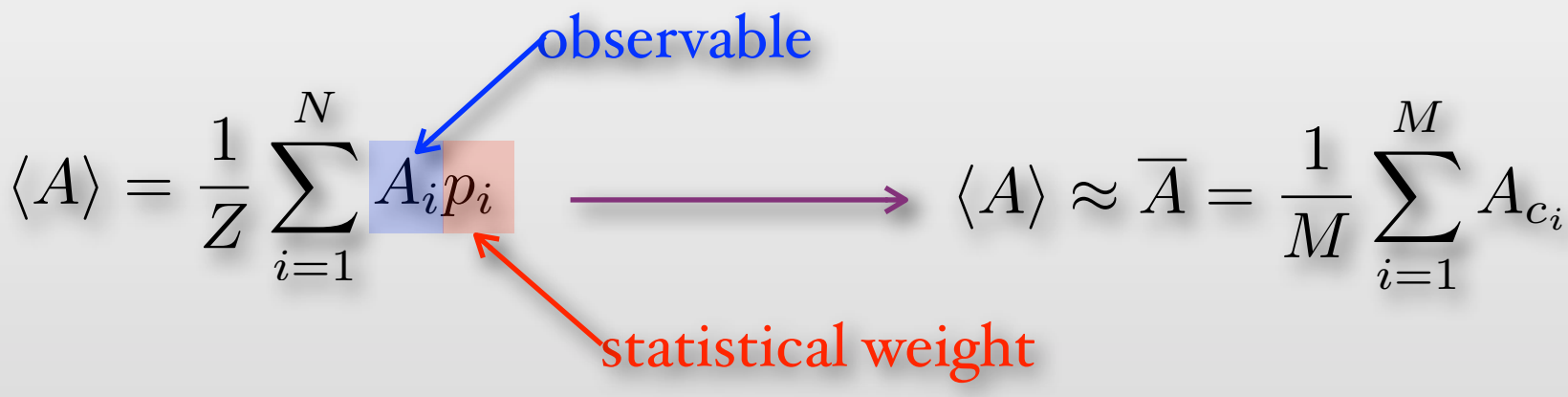
computing in SCIENCE & ENGINEERING

Ulam: the Monte Carlo Method

- What is the probability to win in Solitaire?
  - Ulam's answer: play it 100 times, count the number of wins and you have a pretty good estimate



The Monte Carlo Method



- Need a representative sample with the correct distribution

$$P[c_i] = \frac{p_{c_i}}{Z}$$

  - fundamental problem of statistical mechanics

The Metropolis Algorithm (1953)

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
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(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed,

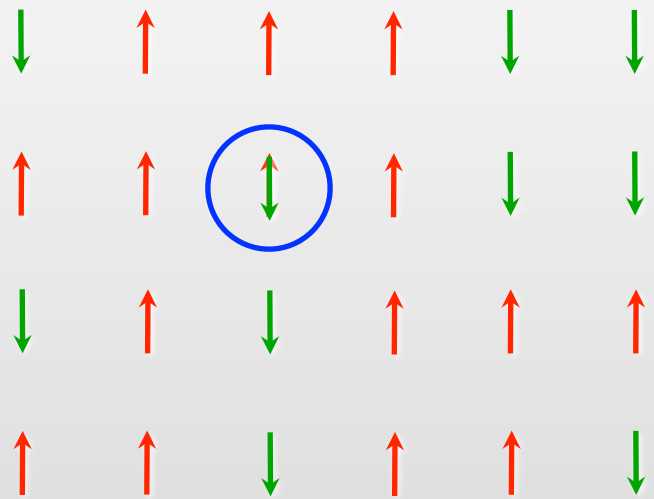
II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number N may be as high as several hundred. Our system consists of a square† con-

I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules.

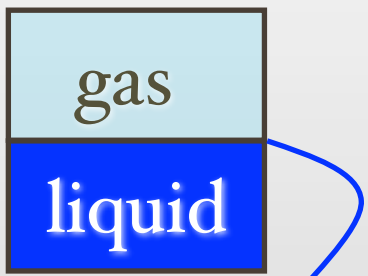
Metropolis algorithm for the Ising model



1. Pick a random spin and propose to flip it
2. Accept the flip with probability $P = \min\left[1, e^{-(E_{new} - E_{old})/T}\right]$
3. Perform a measurement independent of whether the proposed flip was accepted or rejected!

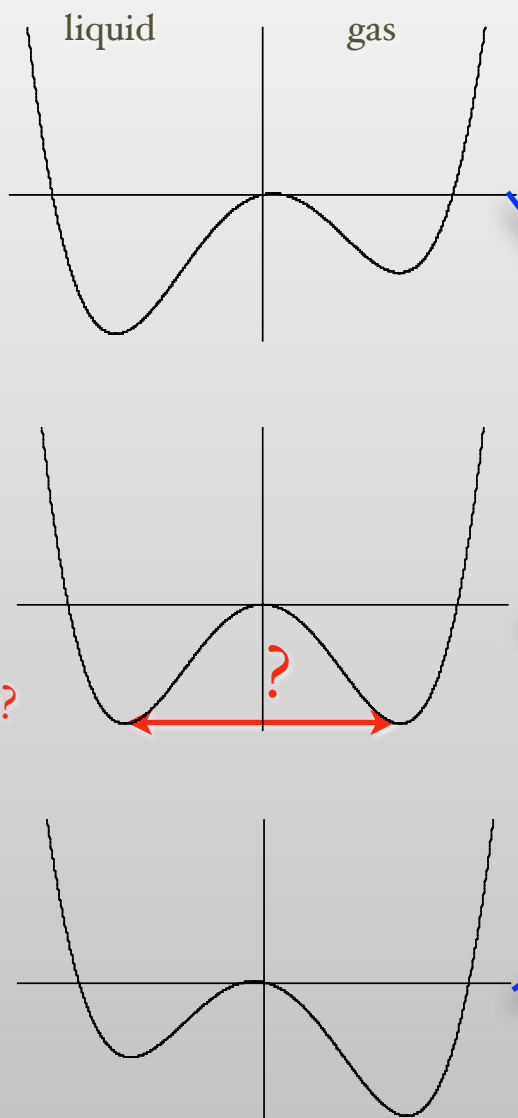
First order phase transitions

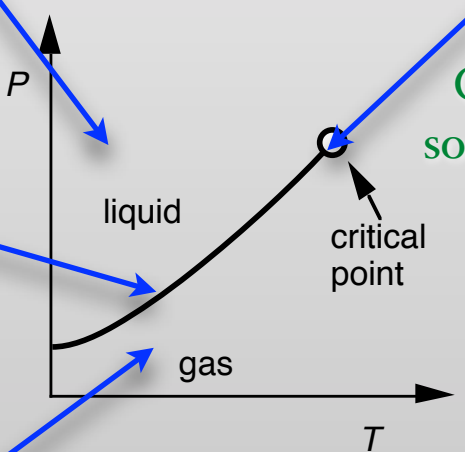
Tunneling out of meta-stable state is suppressed exponentially

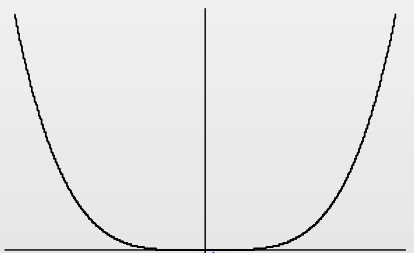


$$\tau \propto \exp(-cL^{d-1}/T)$$

How can we tunnel out of metastable state?



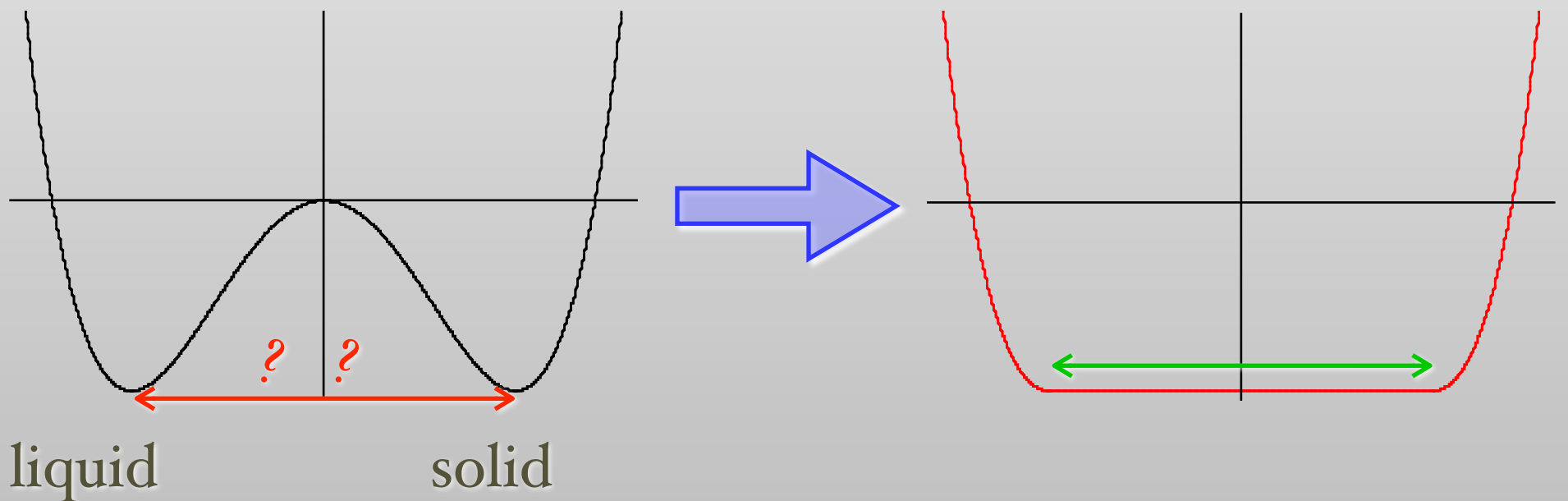




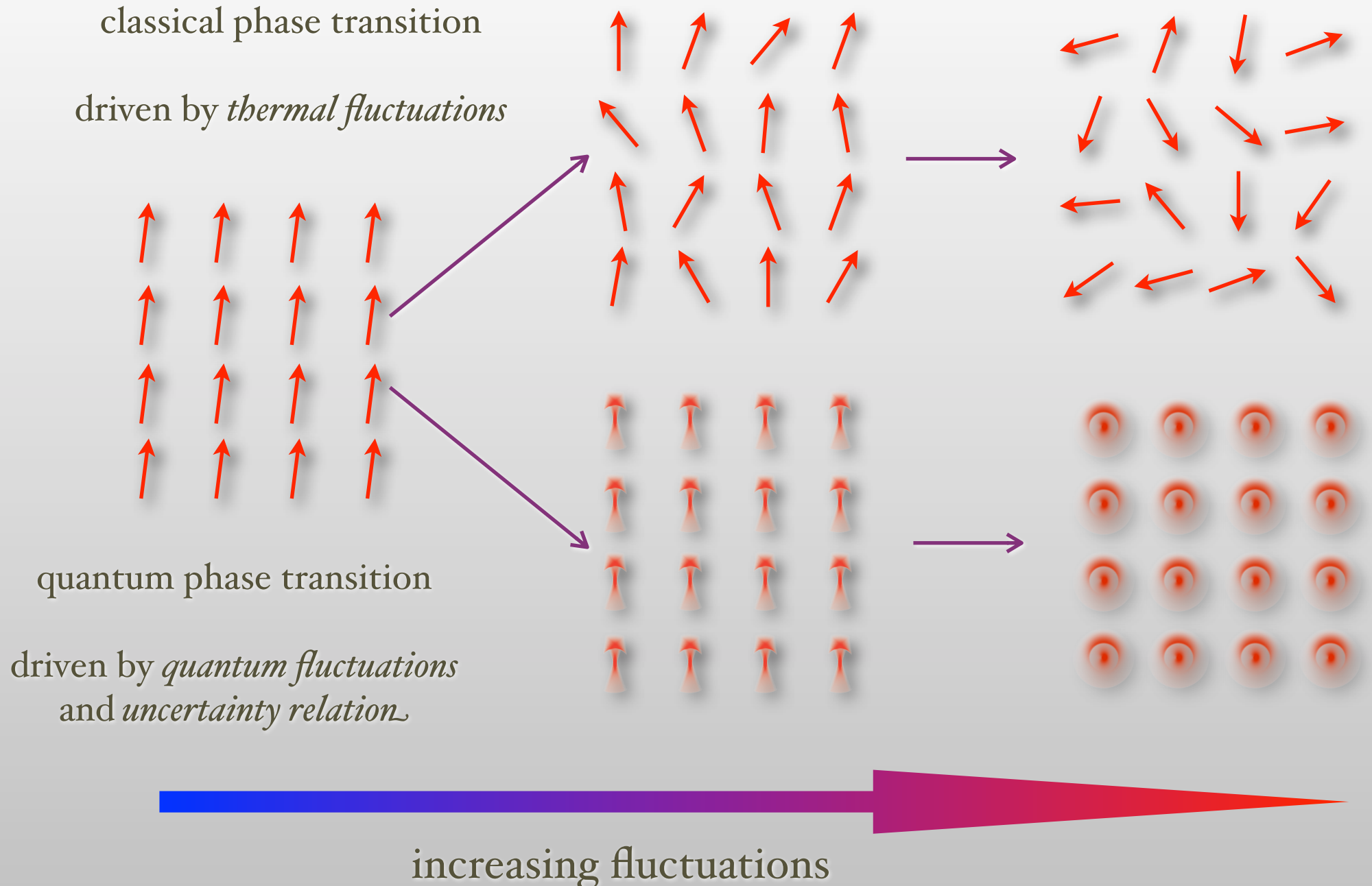
Critical slowing down solved by cluster updates

Modern algorithms

- Critical slowing down at a 2nd order phase transition is solved by *changing the dynamics*: make large global changes
  - Swendsen and Wang, 1987; Evertz *et al*, 1993; Prokof'ev *et al*, 1998
- Tunneling problem at a first order phase transition is solved by *changing the ensemble* to create a flat energy landscape
  - Berg & Neuhaus, 1992; Wang & Landau, 2001; Troyer *et al*, 2003 , ...



Classical and quantum phase transitions

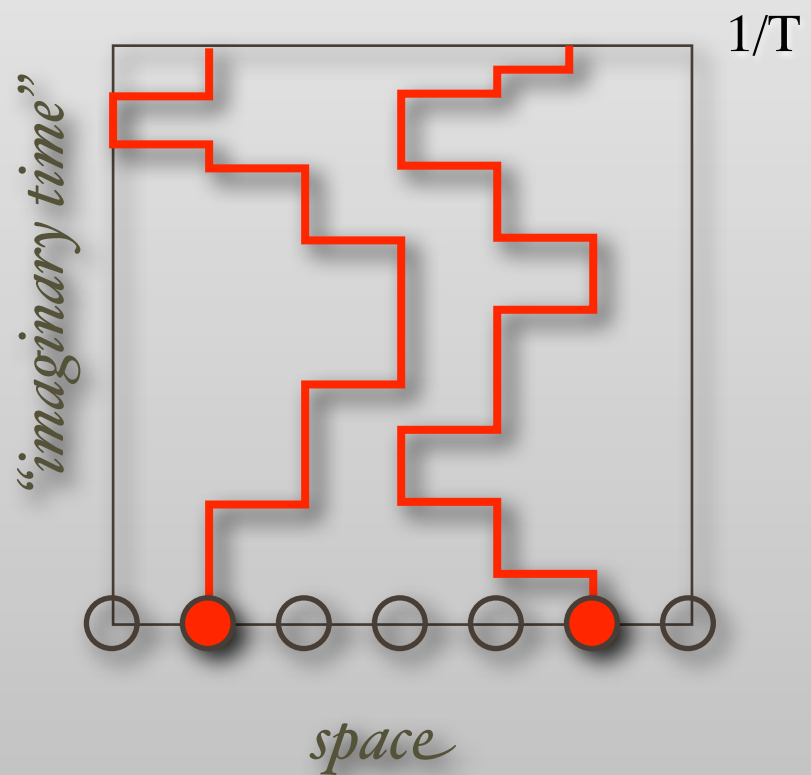


Mapping quantum to classical systems

- Classical: $\langle A \rangle = \sum_c A_c e^{-E_c/T} \Big/ \sum_c e^{-E_c/T}$
- Quantum: $\langle A \rangle = \mathrm{Tr}\, A e^{-H/T} \Big/ \mathrm{Tr}\, e^{-H/T}$
- Calculate exponential by integrating a diffusion equation

$$\frac{d\Psi}{d\tau} = -H\Psi \Rightarrow \Psi(1/T) = e^{-(1/T)H}\Psi(0)$$

- Map to „world lines“ of the trajectories of the particles
- use Monte Carlo samples these world lines



Modern algorithms for quantum systems

- Which system sizes can be studied?

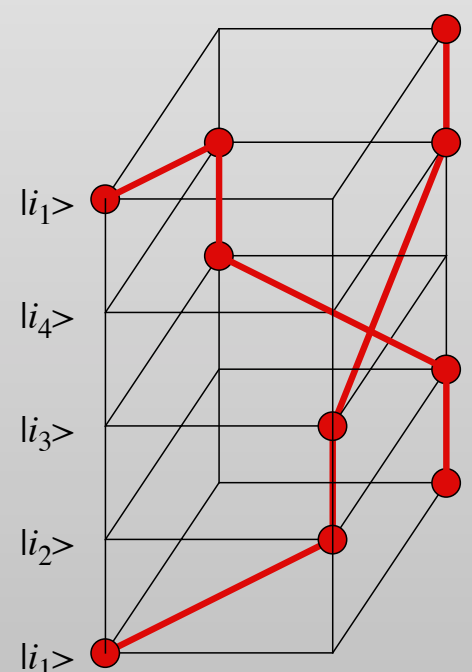
temperature	Metropolis	modern algorithms
3D Tc	16'000 spins	16'000'000 spins
0.1	200 spins	1'000'000 spins
0.005	—	50'000 spins
3D Tc	32 bosons	1'000'000 bosons
0.1	32 bosons	10'000 bosons

The negative sign problem

- In mapping of quantum to classical system

$$Z = \mathrm{Tr} e^{-\beta H} = \sum_i p_i$$

- there is a "sign problem" if some of the $p_i < 0$:
  - Appears e.g. in simulation of electrons when two electrons exchange places (Pauli principle)
- the consequence: exponential scaling!



New phenomena near quantum phase transitions

- Supersolid in Helium-4: can a material be superfluid and solid at the same time?
- Bose-Einstein condensation in ultracold atomic gases and quantum simulators
- Phase diagram of QCD
- These and many other questions will be discussed in the spring in the computational quantum physics lecture

Computational Quantum Physics

- Taught in the spring semester by M. Troyer
  - Solving the one-body Schrödinger equation
  - The many body Schrödinger equation
  - Approximate solutions to the many body Schrödinger equation
    - Quantum chemistry methods
    - Hartree-Fock
    - Density functional theory
  - Exact solutions to the many body Schrödinger equation
    - Path integral quantum Monte Carlo
    - Exact diagonalization
  - Quantum magnets, bosons and fermions
  - Monte Carlo methods for quantum field theories

- Also suitable for RW/CSE students