

# Outline

- 1 Origin of mass
- 2 Thermodynamics & GPU
- 3 Final remark

# The origin of mass of the visible Universe

source of the mass for ordinary matter (not a dark matter talk)

basic goal of LHC (Large Hadron Collider, Geneva Switzerland):

“to clarify the origin of mass”

e.g. by finding the Higgs particle, or by alternative mechanisms  
order of magnitudes: 27 km tunnel and O(10) billion dollars



# The vast majority of the mass of ordinary matter

ultimate (Higgs or alternative) mechanism: responsible for the mass of the leptons and for the mass of the quarks

interestingly enough: just a tiny fraction of the visible mass (such as stars, the earth, the audience, atoms)

electron: almost massless,  $\approx 1/2000$  of the mass of a proton

quarks (in ordinary matter): also almost massless particles

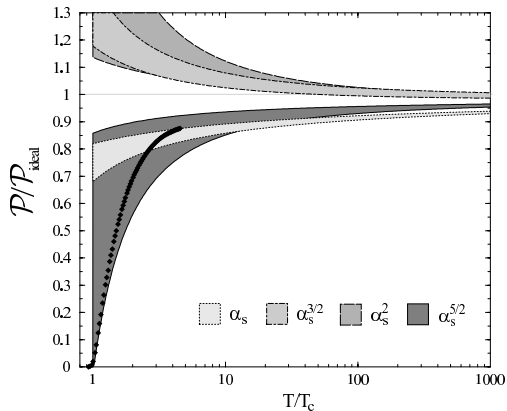
**the vast majority (about 95%) comes through another mechanism**

$\implies$  this mechanism and this 95% will be the main topic of this talk

quantum chromodynamics (QCD, strong interaction) on the lattice

# QCD: need for a systematic non-perturbative method

in some cases: good perturbative convergence; in other cases: bad  
pressure at high temperatures converges at  $T=10^{300}$  MeV



# Lattice field theory

systematic non-perturbative approach (numerical solution):

quantum fields on the lattice

quantum theory: path integral formulation with  $S = E_{kin} - E_{pot}$

quantum mechanics: for all possible paths add  $\exp(iS)$

quantum fields: for all possible field configurations add  $\exp(iS)$

Euclidean space-time ( $t = i\tau$ ):  $\exp(-S)$  sum of Boltzmann factors

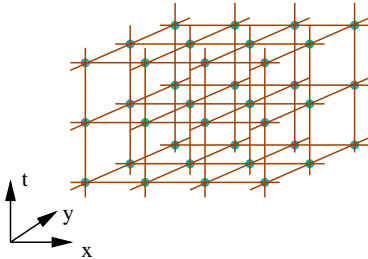
we do not have infinitely large computers  $\Rightarrow$  two restrictions

a. put it on a space-time grid (proper approach: asymptotic freedom)

formally: four-dimensional statistical system

b. finite size of the system (can be also controlled)

$\Rightarrow$  stochastic approach, with reasonable spacing/size: solvable



fine lattice to resolve the  
structure of the proton ( $\lesssim 0.1$  fm)  
few fm size is needed  
50-100 points in 'xyz/t' directions  
 $a \Rightarrow a/2$  means  $100\text{-}200 \times \text{CPU}$



mathematically  
 $10^9$  dimensional integrals  
advanced techniques,  
good balance and  
several Tflops are needed

# Importance sampling

$$Z = \int \prod_{n,\mu} [dU_\mu(n)] e^{-S_g} \det(M[U])$$

we do not take into account all possible gauge configuration

each of them is generated with a probability  $\propto$  its weight

importance sampling, Metropolis algorithm:

(all other algorithms are based on importance sampling)

$$P(U \rightarrow U') = \min [1, \exp(-\Delta S_g) \det(M[U']) / \det(M[U])]$$

gauge part: trace of  $3 \times 3$  matrices (easy, **without M: quenched**)

fermionic part: determinant of  $10^6 \times 10^6$  sparse matrices (hard)

more efficient ways than direct evaluation ( $Mx=a$ ), but still hard

# Hadron spectroscopy in lattice QCD

Determine the transition amplitude between:  
having a “particle” at time 0 and the same “particle” at time  $t$   
 $\Rightarrow$  Euclidean correlation function of a composite operator  $\mathcal{O}$ :

$$C(t) = \langle 0 | \mathcal{O}(t) \mathcal{O}^\dagger(0) | 0 \rangle$$

insert a complete set of eigenvectors  $|i\rangle$

$$= \sum_i \langle 0 | e^{Ht} \mathcal{O}(0) e^{-Ht} | i \rangle \langle i | \mathcal{O}^\dagger(0) | 0 \rangle = \sum_i | \langle 0 | \mathcal{O}^\dagger(0) | i \rangle |^2 e^{-(E_i - E_0)t},$$

where  $|i\rangle$ : eigenvectors of the Hamiltonian with eigenvalue  $E_i$ .

and 
$$\mathcal{O}(t) = e^{Ht} \mathcal{O}(0) e^{-Ht}.$$

$t$  large  $\Rightarrow$  lightest states (created by  $\mathcal{O}$ ) dominate:  $C(t) \propto e^{-M \cdot t}$   
 $t$  large  $\Rightarrow$  exponential fits or mass plateaus  $M_t = \log[C(t)/C(t+1)]$



# Quenched results

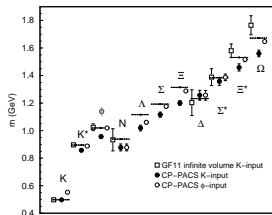
QCD is 35 years old  $\Rightarrow$  properties of hadrons (Rosenfeld table)

non-perturbative lattice formulation (Wilson) immediately appeared  
 needed 20 years even for quenched result of the spectrum (cheap)  
 instead of  $\det(M)$  of a  $10^6 \times 10^6$  matrix trace of  $3 \times 3$  matrices

always at the frontiers of computer technology:

GF11: IBM "to verify quantum chromodynamics" (10 Gflops, '92)

CP-PACS Japanese purpose made machine (Hitachi 614 Gflops, '96)



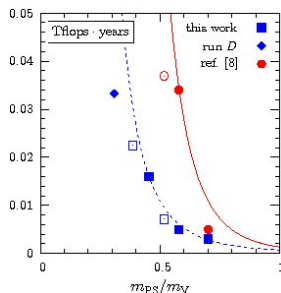
the  $\approx 10\%$  discrepancy was believed to be a quenching effect

# Difficulties of full dynamical calculations

though the quenched result can be qualitatively correct  
uncontrolled systematics  $\Rightarrow$  full “dynamical” studies  
by two-three orders of magnitude more expensive (balance)  
present day machines offer several hundreds of Tflops

no revolution but evolution in the algorithmic developments

Berlin Wall '01: it is extremely difficult to reach small quark masses:



# Ingredients to control systematics

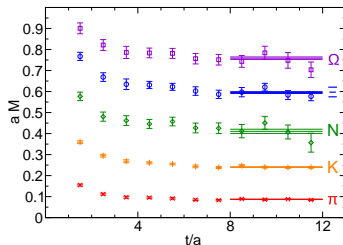
BMW Collaboration, Science 322:1224-1227,2008

- inclusion of  $\det[M]$  with an exact  $n_f=2+1$  algorithm  
action: universality class is known to be QCD (Wilson-quarks)
- spectrum: light mesons, octet & decuplet baryons (resonances)  
(three of these fix the averaged  $m_{ud}$ ,  $m_s$  and the cutoff)
- large volumes to guarantee small finite-size effects  
rule of thumb:  $M_\pi L \gtrsim 4$  is usually used (correct for that)
- controlled interpolations & extrapolations to physical  $m_s$  and  $m_{ud}$   
(or eventually simulating directly at these masses)  
since  $M_\pi \simeq 135$  MeV extrapolations for  $m_{ud}$  are difficult  
CPU-intensive calculations with  $M_\pi$  reaching down to  $\approx 200$  MeV
- controlled extrapolations to the continuum limit ( $a \rightarrow 0$ )  
calculations are performed at no less than 3 lattice spacings

## Scale setting and masses in lattice QCD

in meteorology, aircraft industry etc. grid spacing is set by hand  
 in lattice QCD we use  $g, m_{ud}$  and  $m_s$  in the Lagrangian ('a' not)  
 measure e.g. the vacuum mass of a hadron in lattice units:  $M_\Omega a$   
 since we know that  $M_\Omega = 1672$  MeV we obtain 'a'

masses are obtained by correlated fits (choice of fitting ranges)  
 illustration: mass plateaus at the smallest  $M_\pi \approx 190$  MeV (noisiest)



volumes and masses for unstable particles: avoided level crossing  
 decay phenomena included: in finite V shifts of the energy levels

# Parameters of the Lagrangian

three parameters of the Lagrangian: coupling strength  $g$ ,  $m_{ud}$  and  $m_s$

asymptotic freedom: for large cutoff (small lattice spacing)  $g$  is small  
in this region the results are already independent of  $g$  (scaling)

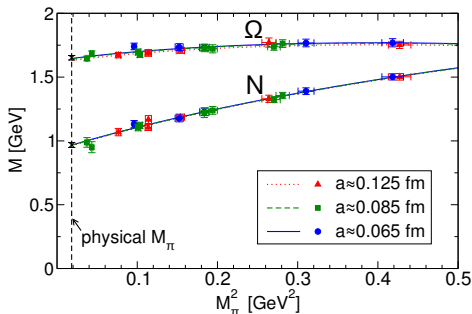
QCD predicts only dimensionless combinations (e.g. mass ratios)  
⇒ we can eliminate  $g$  as an input parameter by taking ratios

the pion mass  $M_\pi$  is particularly sensitive to  $m_{ud}$

the kaon mass  $M_K$  is particularly sensitive to  $m_s$

relatively easy to set the strange quark mass  $m_s$  to its physical value  
it is very CPU demanding to approach the physical  $m_{ud}$

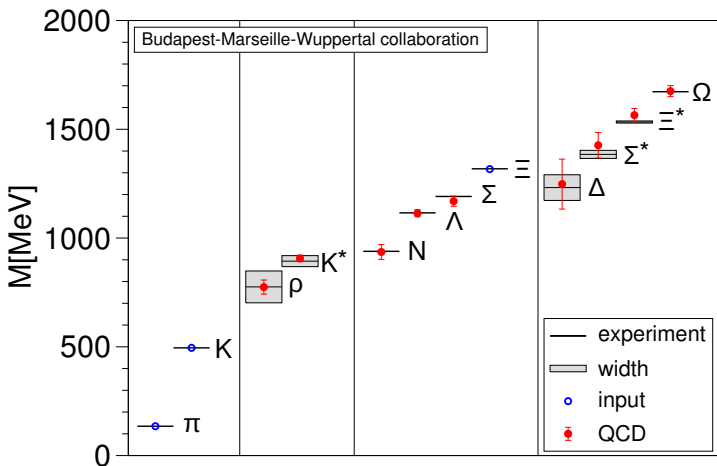
altogether 15 points for each hadrons



smooth extrapolation to the physical pion mass (or  $m_{ud}$ )  
 small discretization effects (three lines barely distinguishable)

continuum extrapolation goes as  $c \cdot a^n$  and it depends on the action  
 in principle many ways to discretize (derivative by 2,3... points)  
 goal: have large  $n$  and small  $c$  (in this case  $n = 2$  and  $c$  is small)

# Final result for the hadron spectrum



## Breakthrough of the Year

# Proton's Mass 'Predicted'

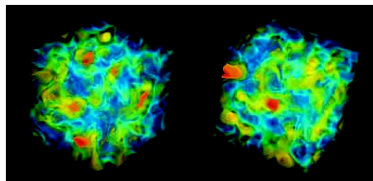
STARTING FROM A THEORETICAL DESCRIPTION OF ITS INNARDS, physicists precisely calculated the mass of the proton and other particles made of quarks and gluons. The numbers aren't new; experimenters have been able to weigh the proton for nearly a century. But the new results show that physicists can at last make accurate calculations of the ultracomplex strong force that binds quarks.

In simplest terms, the proton comprises three quarks with gluons zipping between them to convey the strong force. Thanks to the uncertainties of quantum mechanics, however, myriad gluons and quark-antiquark pairs flit into and out of existence within a

proton in a frenzy that's nearly impossible to analyze but that produces 95% of the particle's mass.

To simplify matters, theorists from France, Germany, and Hungary took an approach known as "lattice quantum chromodynamics."

They modeled continuous space and time as a four-dimensional array of points—the lattice—and confined the quarks to the points and the gluons to the links between them. Using supercomputers, they reckoned the masses of

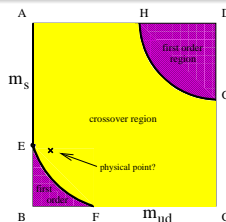


the proton and other particles to a precision of about 2%—a tenth of the uncertainties a decade ago—as they reported in November.

In 2003, others reported equally precise calculations of more-esoteric quantities. But by calculating the familiar proton mass, the new work signals more broadly that physicists finally have a handle on the strong force.



# Phase diagram and its uncertainties



physical quark masses: important for the nature of the transition

$n_f=2+1$  theory with  $m_q=0$  or  $\infty$  gives a first order transition

intermediate quark masses: we have an analytic cross over (no  $\chi$ PT)

F.Karsch et al., Nucl.Phys.Proc. 129 ('04) 614; G.Endrodi et al. PoS Lat'07 182('07);

de Forcrand, S. Kim, O. Philipsen, Lat'07 178('07)

continuum limit is important for the order of the transition:

$n_f=3$  case (standard action,  $N_t=4$ ): critical  $m_{ps} \approx 300$  MeV

different discretization error (p4 action,  $N_t=4$ ): critical  $m_{ps} \approx 70$  MeV

the physical pseudoscalar mass is just between these two values

# Lattice formulation

$$Z = \int dU d\Psi d\bar{\Psi} e^{-S_E} \quad (1)$$

$S_E$  is the Euclidean action

Parameters (the lattice spacing does not appear explicitly):

gauge coupling  $g$

quark masses  $m_i$  ( $i = 1..N_f$ )

(Chemical potentials  $\mu_i$ )

Volume ( $V$ ) and temperature ( $T$ )

Finite  $T \leftrightarrow$  finite temporal lattice extension

$$T = \frac{1}{N_t a} \quad (2)$$

Continuum limit:  $a \rightarrow 0 \iff N_t \rightarrow \infty$ ; CPU demand scales as  $N_t^{8-12}$

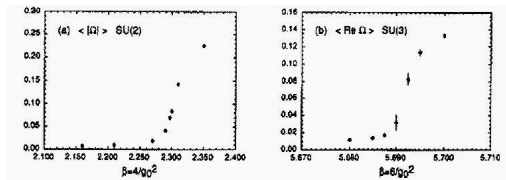
# Finite-size scaling theory

## problem with phase transitions in Monte-Carlo studies

Monte-Carlo applications for pure gauge theories ( $V = 24^3 \cdot 4$ )

existence of a transition between confining and deconfining phases:

Polyakov loop exhibits rapid variation in a narrow range of  $\beta$



• theoretical prediction: SU(2) second order, SU(3) first order

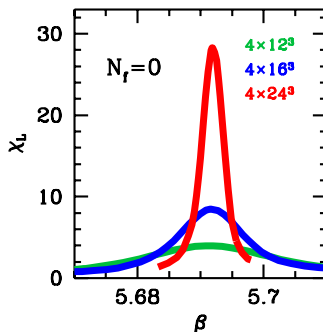
⇒ Polyakov loop behavior: SU(2) singular power, SU(3) jump

data do not show such characteristics!

# Finite size scaling in the quenched theory

look at the susceptibility of the Polyakov-line

first order transition (Binder)  $\Rightarrow$  peak width  $\propto 1/V$ , peak height  $\propto V$



finite size scaling shows: the transition is of first order

# The nature of the QCD transition

Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675

finite size scaling study of the chiral condensate (susceptibility)

$$\chi = (T/V) \partial^2 \log Z / \partial m^2$$

**phase transition:** finite  $V$  analyticity  $V \rightarrow \infty$  increasingly singular

(e.g. first order phase transition: height  $\propto V$ , width  $\propto 1/V$ )

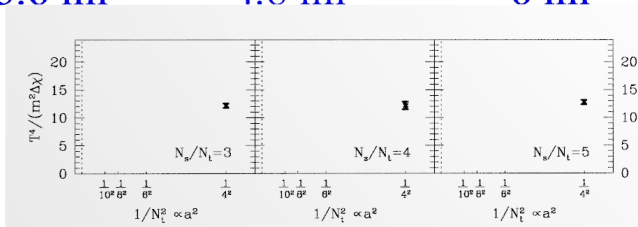
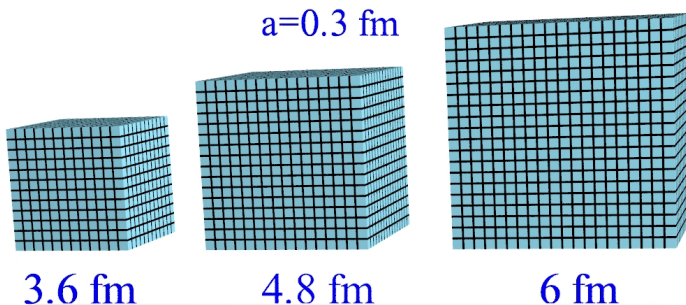
for an **analytic** cross-over  $\chi$  **does not grow with  $V$**

two steps (three volumes, four lattice spacings):

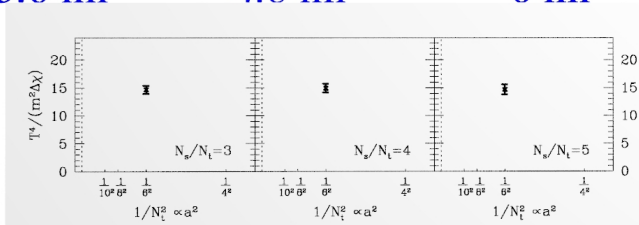
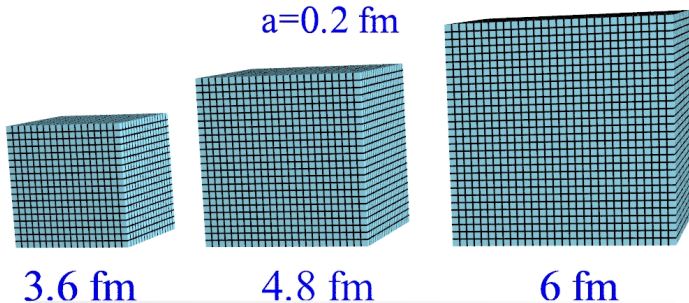
a. **fix  $V$  and determine  $\chi$  in the continuum limit:**  $a=0.3, 0.2, 0.15, 0.1 \text{ fm}$

b. using the continuum extrapolated  $\chi_{max}$ : **finite size scaling**

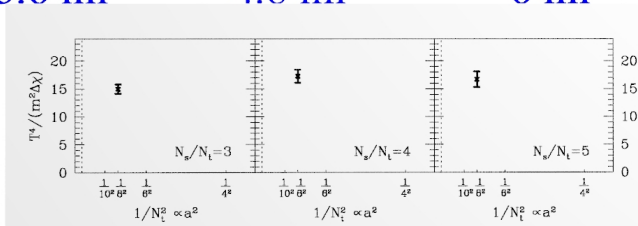
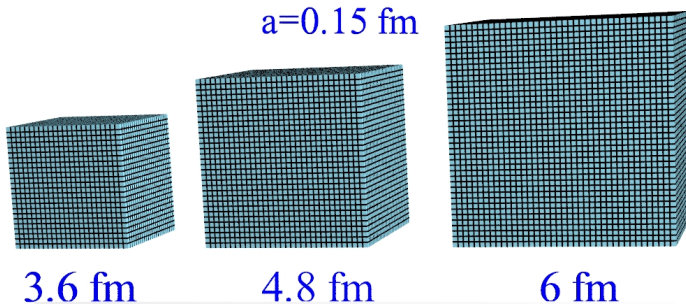
# Approaching the continuum limit



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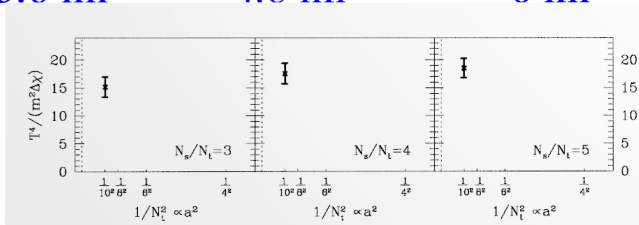
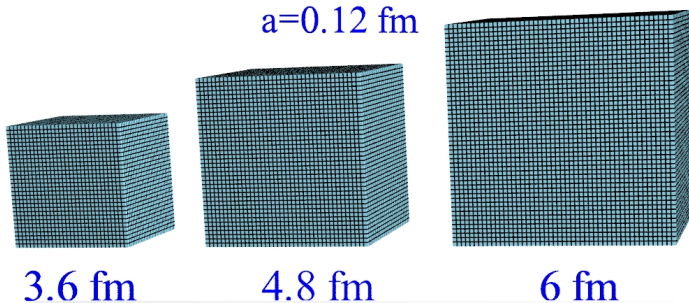


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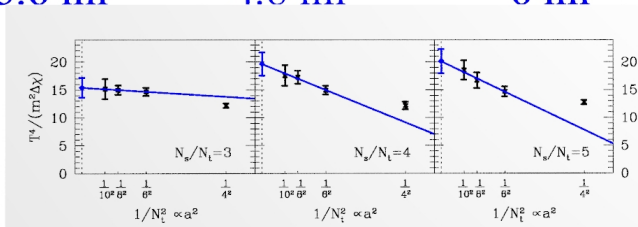
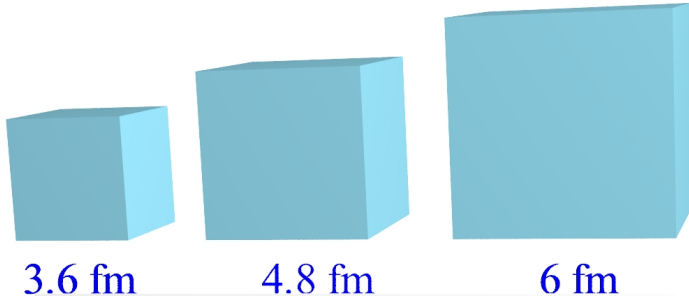




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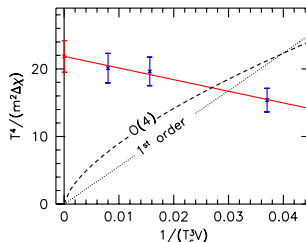


# Approaching the continuum limit



# The nature of the QCD transition: analytic

- finite size scaling analysis with continuum extrapolated  $T^4/m^2\Delta\chi$



the result is consistent with an approximately constant behavior for a factor of 5 difference within the volume range  
 chance probability for  $1/V$  is  $10^{-19}$  for  $O(4)$  is  $7 \cdot 10^{-13}$   
 continuum result with physical quark masses in staggered QCD:

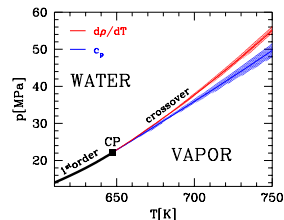
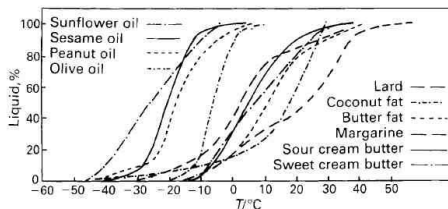
**the QCD transition is a cross-over**

# The nature of the QCD transition

Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675

**analytic transition (cross-over)**  $\Rightarrow$  it has no unique  $T_c$ :

examples: melting of butter (not ice) & water-steam transition

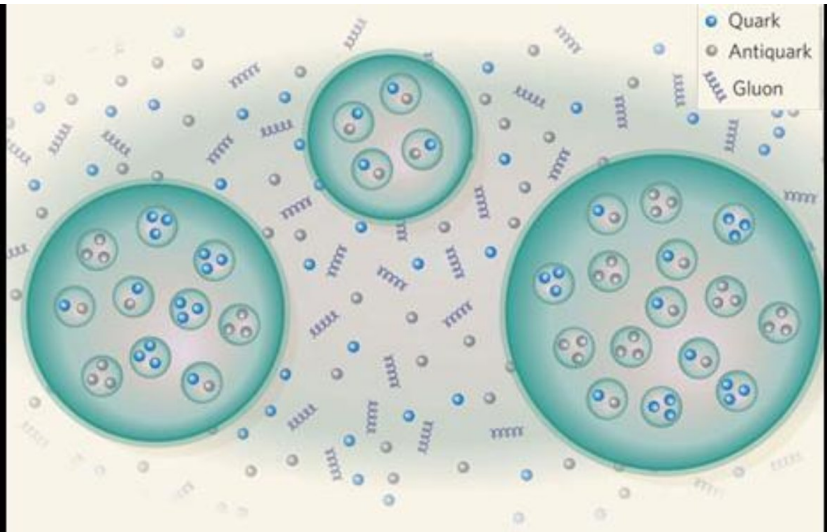


above the critical point  $c_p$  and  $d\rho/dT$  give different  $T_c$ s.

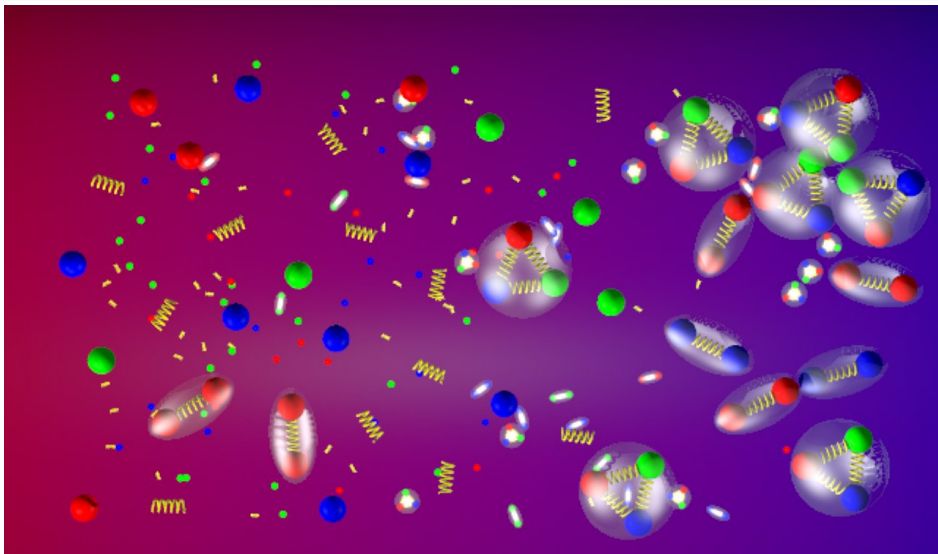
**QCD: chiral & quark number susceptibilities or Polyakov loop**

they result in different  $T_c$  values  $\Rightarrow$  physical difference

# Possible first order scenario with critical bubbles



# Reality: smooth analytic transition (cross-over)



# Historical background

1972 Lagrangian of QCD (H. Fritzsch, M. Gell-Mann, H. Leutwyler)

1973 asymptotic freedom (D. Gross, F. Wilczek, D. Politzer)  
at small distances (large energies) the theory is “free”

1974 lattice formulation (Kenneth Wilson)  
at large distances the coupling is large: non-perturbative

Nobel Prize 2008: Y. Nambu, & M. Kobayashi T. Masakawa

spontaneous symmetry breaking in quantum field theory  
strong interaction picture: mass gap is the mass of the nucleon

mass eigenstates and weak eigenstates are different

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## Scientific Background on the Nobel Prize in Physics 2008

“Even though QCD is the correct theory for the strong interactions, it can not be used to compute at all energy and momentum scales ... (there is) ... a region where perturbative methods do not work for QCD.”

true, but the situation is somewhat better: new era  
fully controlled non-perturbative approach works (took 35 years)