

# The phase diagram of strong interactions from lattice QCD simulations

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Many aspects of strong interactions require a treatment of QCD in the low energy regime, where the coupling constant is large and perturbation theory fails.

- **Color Confinement:** why are color degrees of freedom, quarks and gluons, not visible in Nature and instead confined into hadrons?
- **Chiral Symmetry Breaking ( $\chi$ SB):** why the ground state of QCD breaks part of the flavor symmetry group spontaneously?
- Is **confinement** (and  $\chi$ SB) a permanent state of matter? Do new phases emerge in unusual conditions (temperature, density, ...) reproduced somewhere-when in the Universe? (Cabibbo, Parisi, 1975)
- Can we predict the nature of the different possible phases and of the transitions among them? **QCD Phase Diagram**

**In absence of a systematic, quantitatively reliable analytic approaches to non-perturbative QCD, a numerical treatment is the best present first-principle approach**

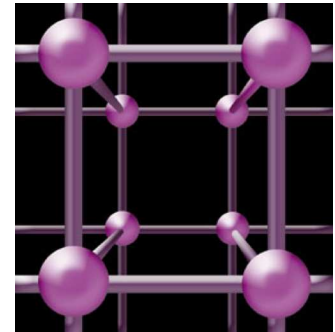
**The starting point is the path-integral approach to Quantum Mechanics and Quantum Field Theory, opened by R. Feynman in 1948.**

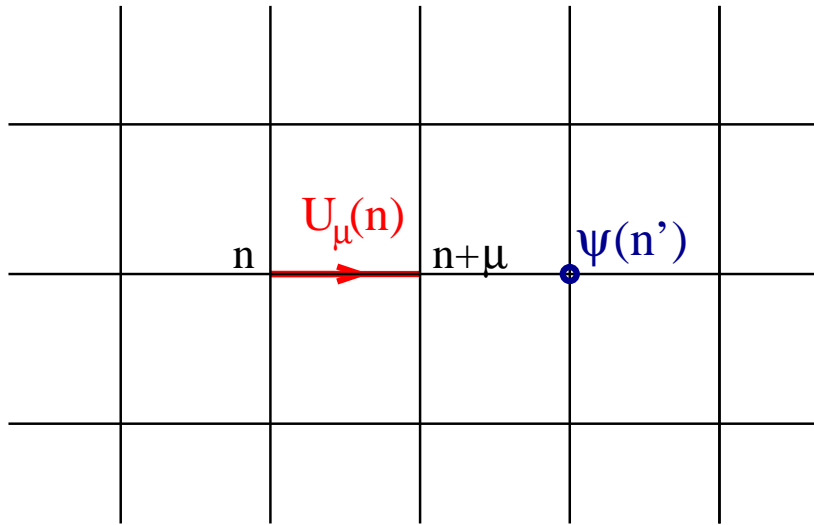
$$\langle 0|O|0\rangle \Rightarrow \int \mathcal{D}\varphi e^{-S[\varphi]} O[\varphi]$$

**The QCD path integral is discretized on a finite space-time lattice  
 $\Rightarrow$  finite number of integration variables**

**The path-integral is then computed by Monte-Carlo algorithms which samples field configurations  $\varphi(\vec{x}, t)$  proportionally to  $e^{-S[\varphi]}$**

$$\int \mathcal{D}\varphi e^{-S[\varphi]} O[\varphi] \simeq \bar{O} = \frac{1}{M} \sum_{i=1}^M O[\varphi_i]$$





In lattice QCD, elementary variables are  $3 \times 3$  unitary complex matrixes living on lattice links (**link variables**)

$$U_\mu(n) \simeq \mathcal{P} \exp \left( ig \int_n^{n+\mu} A_\mu dx_\mu \right)$$

**Fermion fields live on lattice sites**

The thermal QCD partition function is rewritten in terms of an Euclidean path integral

$$Z(V, T) = \text{Tr} \left( e^{-\frac{H_{\text{QCD}}}{T}} \right) \Rightarrow \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-(S_G[U] + \bar{\psi} M[U] \psi)} = \int \mathcal{D}U e^{-S_G[U]} \det M[U]$$

As long as  $\mathcal{D}U e^{-S_G} \det M[U]$  is positive, it can be interpreted as a probability distribution  $\mathcal{D}U \mathcal{P}[U]$  over gauge link configurations.



$$T = \frac{1}{\tau} = \frac{1}{N_t a(\beta, m)}$$

$\tau$  is the extension of the compactified time

Sample averages give access to equilibrium properties: energy density, specific heat, particle number susceptibilities and other quantities needed to locate the transition, study its order, study the properties of different phases (e.g. equation of state)

## Uncertainties

- **statistical:** finite sample, error  $\sim 1/\sqrt{\text{sample size}}$ .
- **systematic:** finite box size  $L$ , finite lattice spacing  $a$ , unphysical quark masses.

Given enough computer power, uncertainties can be kept under control. Results from different groups, adopting different discretizations, converge to consistent results.

Projects employing  $L \gg 1$  fm,  $a$  well below 0.1 fm and physical quark masses, require more than 100 Teraflop\*year (**almost  $10^{22}$  floating point operations**)

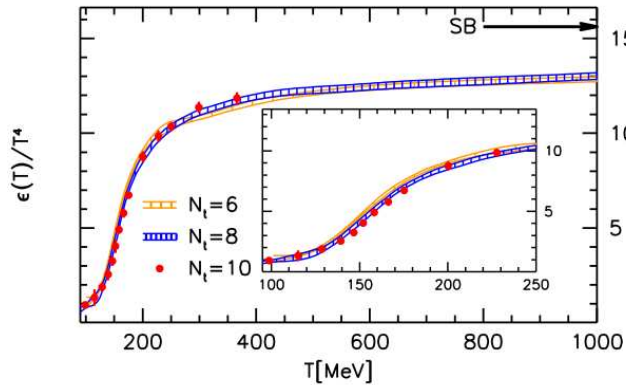
## Finite T transition

The liberation of color degrees of freedom is clearly visible in thermodynamical quantities and coincides with chiral symmetry restoration.

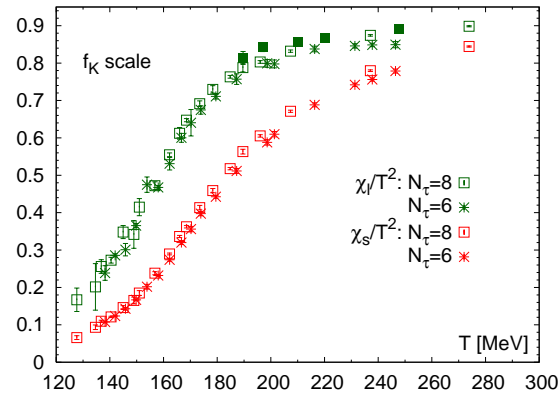
energy density

$u/d$  and  $s$  number fluctuations

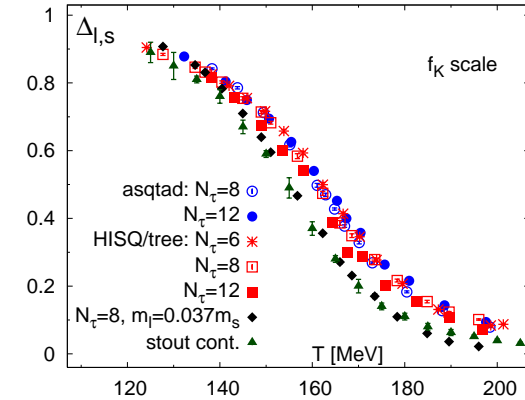
chiral condensate



arXiv:1007.2580



arXiv:1111.1710



arXiv:1111.1710

## Temperature and nature of the transition (from the chiral condensate)

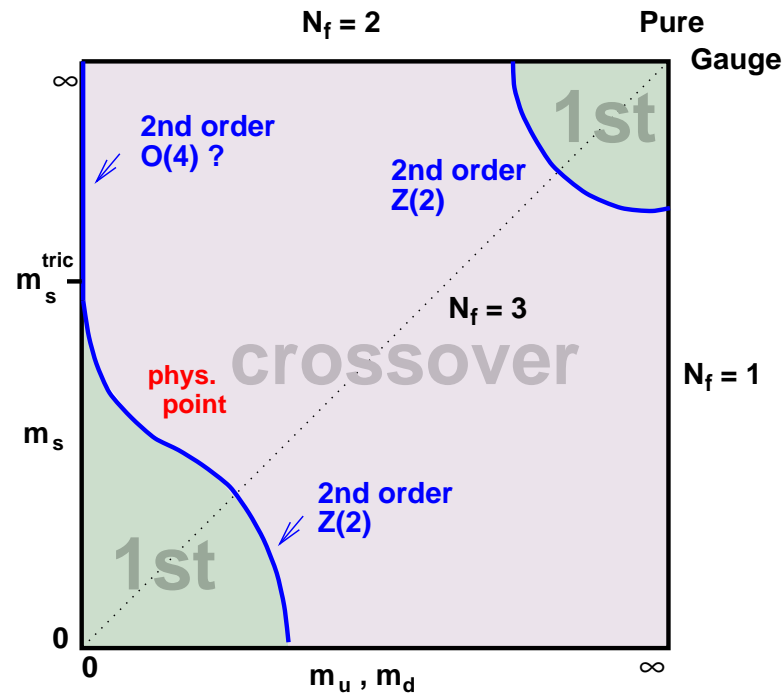
S. Borsanyi *et al.* JHEP 1009, 073 (2010)  $T_c = 155(6)$  MeV (stout link stag. discretization,  $a_{min} \simeq 0.08$  fm)

A. Bazavov *et al.*, PRD 85, 054503 (2012)  $T_c = 154(9)$  MeV (HISQ/tree stag. discretization,  $a_{min} \simeq 0.1$  fm)

The physical point is consistent with a crossover (no discontinuity) (Aoki *et al.*, Nature 443, 675 (2006)): either the transition is extremely weak (hence not phenomenologically relevant) or absent

# In numerical simulations the quark mass spectrum can be changed at will

It makes sense to study the nature of the transition as a function of  $u/d$  and  $s$  quark masses



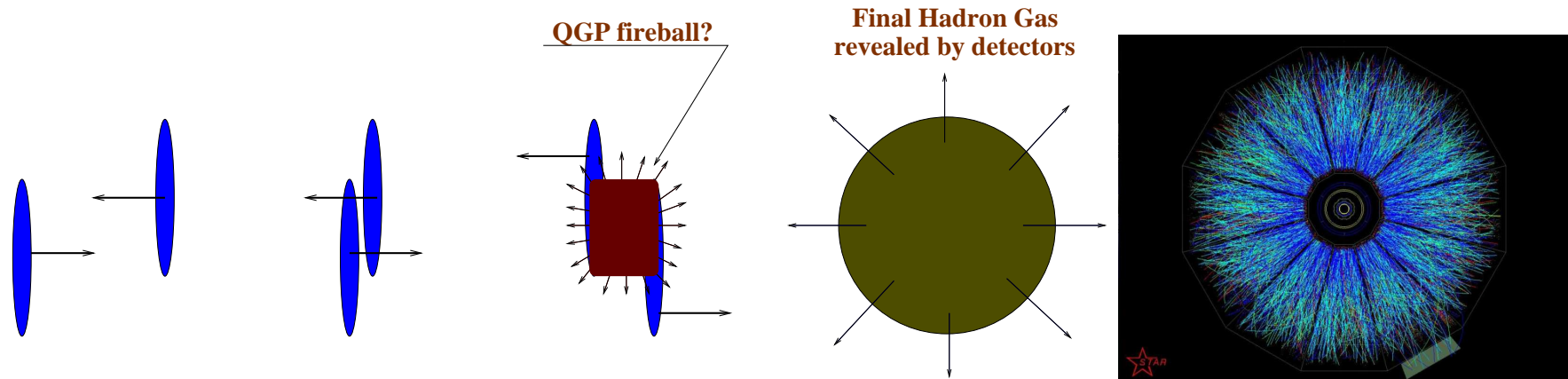
← COLUMBIA PLOT

A true, first order transition is present for very light or very heavy quark masses

Unsettled issues in the chiral limit of  $N_f = 2$ : 2nd order or first order?

(Bonati, Cossu, M.D., Di Giacomo, Pica, '05, '07, in progress; Bonati, M.D., de Forcrand, Philipsen, Sanfilippo, '11, in progress)

# Experimental input? Heavy Ion Collisions (SPS, RHIC, LHC, ... FAIR)



- Only final products directly accessible, particle multiplicities and ratios are well described by thermal distribution reached at chemical freeze-out like for Cosmic Microwave Background after Big Bang

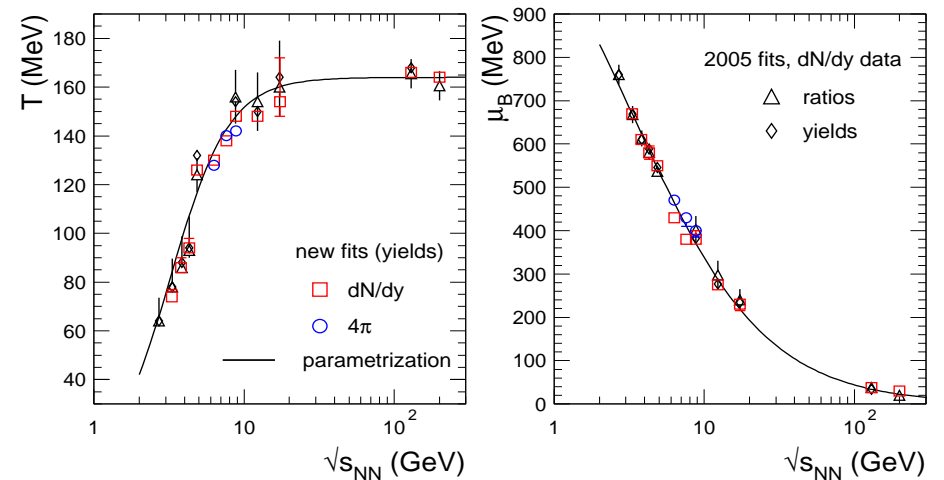
Depending on the c.m. energy, different values of

$T$  and  $\mu_B$  reached at freeze-out:

$\mu_B \sim O(100)$  MeV at SPS, FAIR;  $\mu_B \sim O(10)$

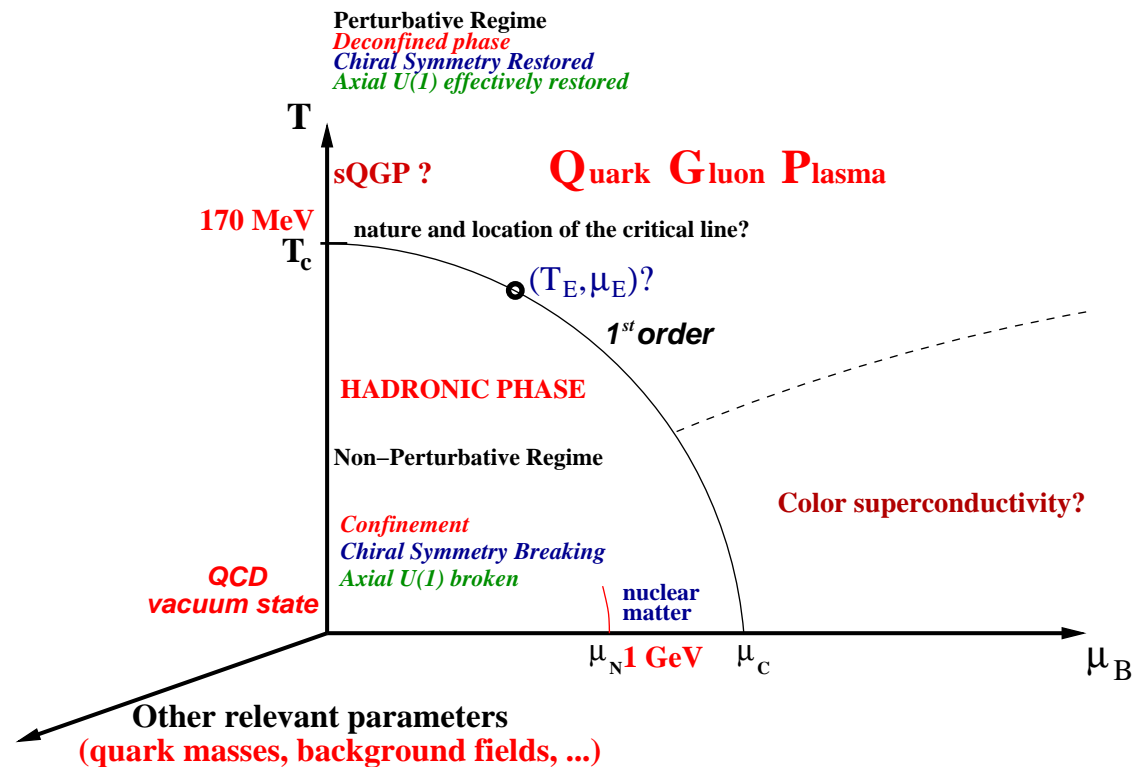
MeV at RHIC;  $\mu_B \sim O(1)$  MeV at LHC;  $\mu_B/T \sim$

$10^{-9}$  at the cosmological transition





## The QCD phase diagram: not just temperature ...



### What we would like to know:

- Location and nature of deconfinement/chiral symmetry restoration as a function of other external parameters ( $\mu_B$ , external fields, ...)
- If crossover at  $\mu_B = 0$  and first order at large  $\mu_B$ : **QCD critical endpoint**  
**Is it there? Where?** (would have clear experimental signatures)
- Location and properties of other exotic phases

## Problems in lattice QCD at $\mu_B \neq 0$

$$Z(\mu_B, T) = \text{Tr} \left( e^{-\frac{H_{\text{QCD}} - \mu_B N_B}{T}} \right) = \int \mathcal{D}U e^{-S_G[U]} \det M[U, \mu_B]$$

$\det M[\mu_B]$  **complex**  $\implies$  **Monte Carlo simulations are not feasible.**

This is usually known as the **sign problem**.

We can then rely on a few approximate methods, viable only for small  $\mu_B/T$ , like

- **Taylor expansion of physical quantities around  $\mu = 0$**

Bielefeld-Swansea collaboration 2002; R. Gavai, S. Gupta 2003

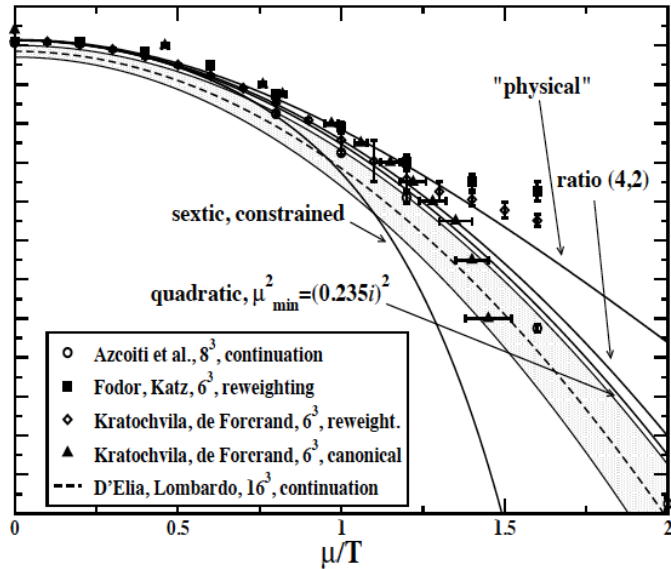
- **Rewighting (complex phase moved from the measure to observables)**

Barbour et al. 1998; Z. Fodor and S. Katz, 2002

- **Simulations at imaginary chemical potentials (plus analytic continuation)**

Alford, Kapustin, Wilczek, 1999; de Forcrand, Philipsen, 2002; M.D'E., Lombardo 2003.

## An example: the critical line $T_c(\mu_B)$



Comparison of various methods to extract  $T_c(\mu_B)/T_c(0)$  as a function of  $\mu_B$  (4 stag. flavors)

P. Cea, L. Cosmai, M. D'E., A. Papa, PRD 81, 094502 (2010).

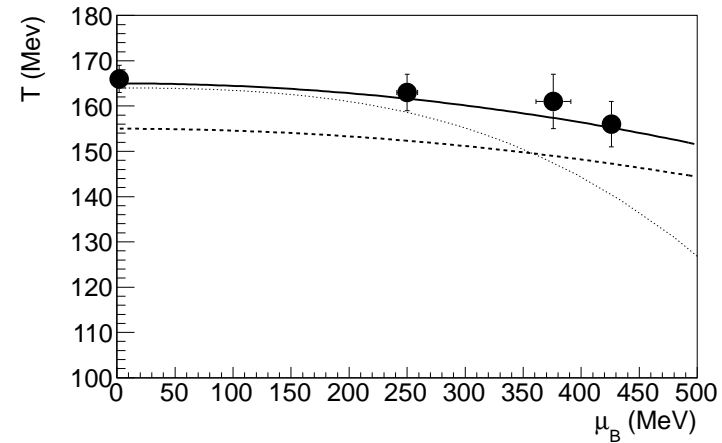
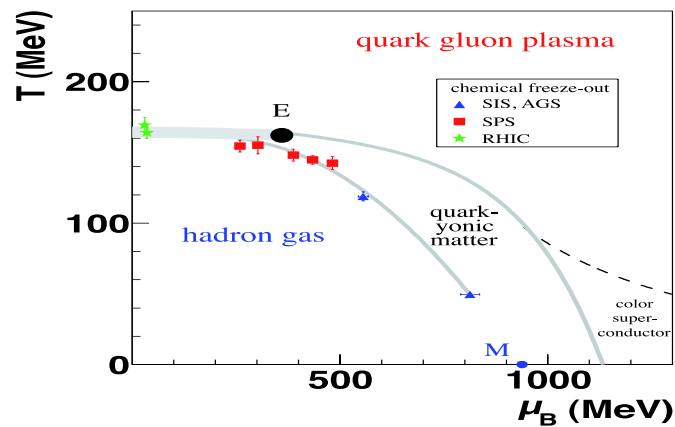
Various different methods agree for the curvature  $\partial T/\partial \mu^2$  of the critical line at  $\mu^2 = 0$ .

In more physical cases we obtain for the curvature  $T_c(\mu_q)/T_c(0) = 1 - A \left(\frac{\mu_q}{T}\right)^2$

- $A = 0.051(4)$  ( $N_f = 2$ ,  $m_\pi \sim 280$  MeV, analytic cont., de Forerand, Philipsen, hep-lat/0205016)
- $A = 0.052(2)$  (as above,  $m_\pi \sim 400$  MeV Cea, Cosmai, D'E., Papa, Sanfilippo, arXiv:1202.5700)
- $A = 0.059(2)(4)$  ( $N_f = 2+1$ , chiral+continuum limit, Taylor, O. Kaczmarek *et al.* arXiv:1011.3130)
- $A = 0.07-0.09$  ( $N_f = 2 + 1$ , physical point, Taylor, G. Endrodi *et al.* arXiv:1102.1356)

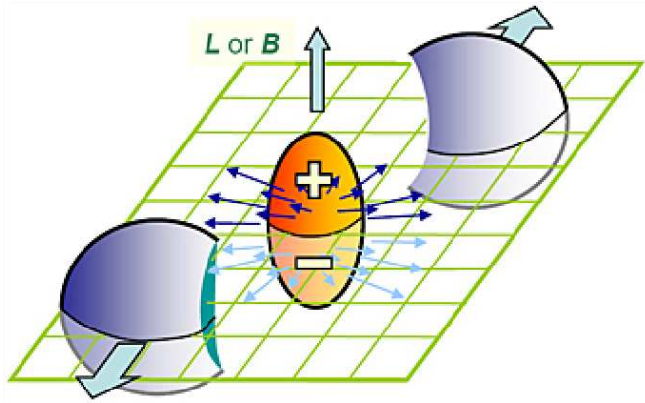
Systematics get out of control at larger  $\mu_B$ , with large uncertainties regarding the location and the very existence of a possible QCD critical endpoint.

## Freeze-out curves and the critical line from lattice QCD



- The freeze out curve seems to be systematically below the transition line determined by lattice QCD:  $A \sim 0.2$  from freeze-out,  $A \sim 0.05$  from lattice (left)
- No a priori reason for the two lines to coincide: hadrons interact even after the parton  $\rightarrow$  hadron transition. However, the gap leaves space for speculations about new possible phases, like the "Quarkyonic Phase" (McLerran, Pisarsky, 2007)
- **Latest News:** a recent reanalysis (right), taking into account baryon-antibaryon annihilation after freeze-out, seems to bring the freeze-out curve on top of lattice data! (F. Becattini *et al*, arXiv:1212.2431)

## Strong interactions in strong magnetic fields



- in non-central heavy ion collisions, largest magnetic fields ever created ( $B$  up to  $10^{15}$  Tesla at LHC)

- possible strong fields in the early Universe, at the time of the QCD transition ( $B$  up to  $10^{16}$  Tesla)

- Possible interplay between  $\vec{B}$  and CP-violating solutions of Yang-Mills theory (**instantons**), may be revealable experimentally by anomalous electric charge fluctuations with respect to the reaction plane: **CHIRAL MAGNETIC EFFECT**  
(A. Vilenkin, 1980, D. E. Kharzeev, L. D. McLerran and H. J. Warringa, K. Fukushima, 2008)
- Recent lattice simulations have shown that strong magnetic fields can have significant effects on the location and on the nature of the phase transition  
M. D., S. Mukherjee, F. Sanfilippo, PRD 82, 051501 (2010); G. S. Bali *et al*, JHEP 1202, 044 (2012).
  - $T_c$  decreases as a function of  $B$
  - the strength of the transition increases as a function of  $B$

## CONCLUSIONS AND ADDENDA

- Present computational resources permit to obtain consistent predictions about the phase diagram of strong interactions, based on the first principles of QCD
- Some cases exist where we still do not have full control systematic errors, like QCD at large baryon density or the computation of transport coefficients, and where major progress could be achieved by future breakthroughs.
- There are fundamental questions needing more theoretical efforts: **which mechanism drives confinement/deconfinement and what its relation to  $\chi$ SB?**

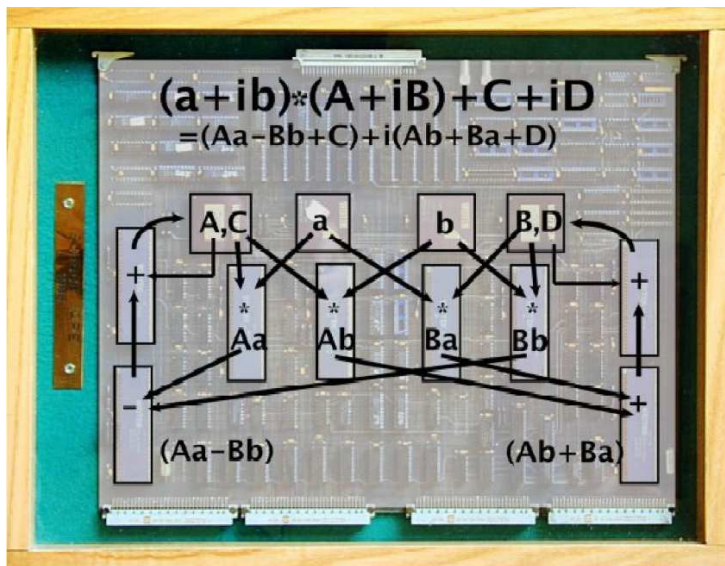
The general idea is that the mechanism is linked to topological objects of dual nature (monopoles, instantons, vortices, ...) and their condensation. Lattice simulations are providing some evidence about that.

(see, e.g., J. Greensite, hep-lat/0301023; C. Bonati, G. Cossu, M.D., A. Di Giacomo, arXiv:1111.1541; A. D'Alessandro, M.D., E. Shuryak, arXiv:1002.4161)

## Computational resources: which, when and where

Lattice QCD simulations are ideally suited for parallelization and have been a major stimulus for the development of High Performance Computing resources.

An example is the series of APE machines "made in INFN"



first APE project, 1988, 250 Mflops



APEnext, 2006, 10 Tflops

Many supercomputer facilities are today at the Petaflop ( $10^{15}$  flops) scale, opening the way to precision lattice computations of strong interaction physics.

# Major computational resources for Lattice QCD in Italy today

## - A share on the 2 Petaflop BlueGene/Q machine at CINECA:



The following table gives the Top 10 positions of the 40th TOP500 List released on November 12, 2012.

Rank	Rmax Rpeak (Pflops)	Name	Computer design Processor type, interconnect	Vendor	Site Country, year	Operating system
1	17,590 27,113	<i>Titan</i>	Cray XK7 16 core AMD Opteron CPU + Nvidia K20 GPU, Custom	Cray	Oak Ridge National Laboratory (ORNL) in Tennessee United States, 2012	Cray Linux Env (SuSE based)
2	16,325 20,133	<i>Sequoia</i>	Blue Gene/Q PowerPC A2, Custom	IBM	Lawrence Livermore National Laboratory United States, 2011	Linux (RHEL and CNK)
3	10,510 11,280	<i>K computer</i>	RIKEN SPARC64 VIII/x, Tofu	Fujitsu	RIKEN Japan, 2011	Linux
4	8,162 10,066	<i>Mira</i>	Blue Gene/Q PowerPC A2, Custom	IBM	Argonne National Laboratory United States, 2012	Linux (RHEL and CNK)
5	4,141 5,033	<i>JUQUEEN</i>	Blue Gene/Q PowerPC A2, Custom	IBM	Forschungszentrum Jülich Germany, 2012	Linux (RHEL and CNK)
6	2,897 3,185	<i>SuperMUC</i>	iDataPlex DX360M4 Xeon E5-2680, Infiniband	IBM	Leibniz-Rechenzentrum Germany, 2012	Linux
7	2,660 3,959	<i>Stampede</i>	iDataPlex DX360M4 Xeon E5-2680, Infiniband	Dell	Texas Advanced Computing Center United States, 2012	Linux
8	2,566 4,701	<i>Tianhe-1A</i>	NUDT YH Cluster Xeon 5670 + Tesla 2050, Arch <sup>61</sup>	NUDT	National Supercomputing Center of Tianjin China, 2010	Linux
9	1,725 2,097	<i>Fermi</i>	Blue Gene/Q Power BQC 16C, Custom	IBM	CINECA Italy, 2012	Linux (RHEL and CNK)
10	1,515 1,944	<i>DARPA Trial Subset</i>	Power 775, Custom	IBM	IBM Development Engineering United States, 2012	Linux

- GPUs: provide O(1) Teraflop cheap power on a Graphic Card
- Dedicated GPU clusters at INFN-PISA, INFN-ROME (QUONG), INFN-GENOVA



- CNS4-cluster at INFN-PISA

- EURORA machine at CINECA (to be installed)

- FUTURE?: Progetto Premiale INFN "SUMA"