

# Phase diagram, fluctuations, thermodynamics and hadron chemistry

Observables and concepts

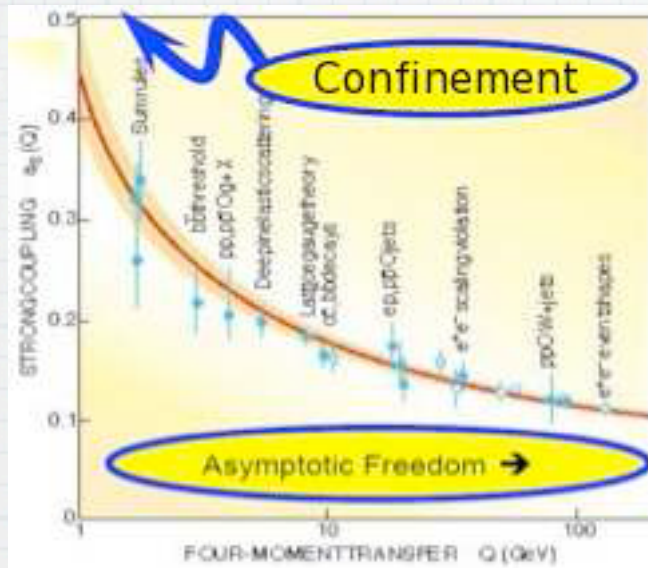
---

**Claudia Ratti**

University of Torino and INFN Torino (ITALY)



# QCD Thermodynamics

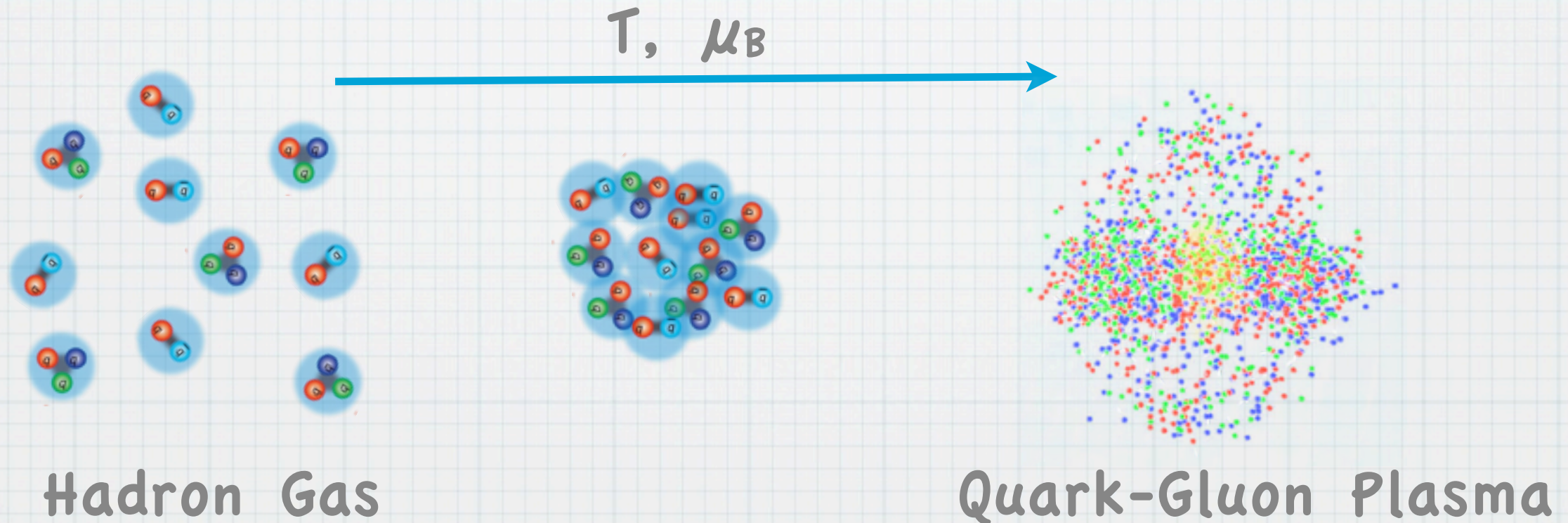


## \* Confinement

- \* At large distances the effective coupling is large
- \* Free quarks are not observed in nature

## \* Asymptotic freedom

- \* At short distances the effective coupling decreases
- \* Quarks and gluons appear to be quasi-free

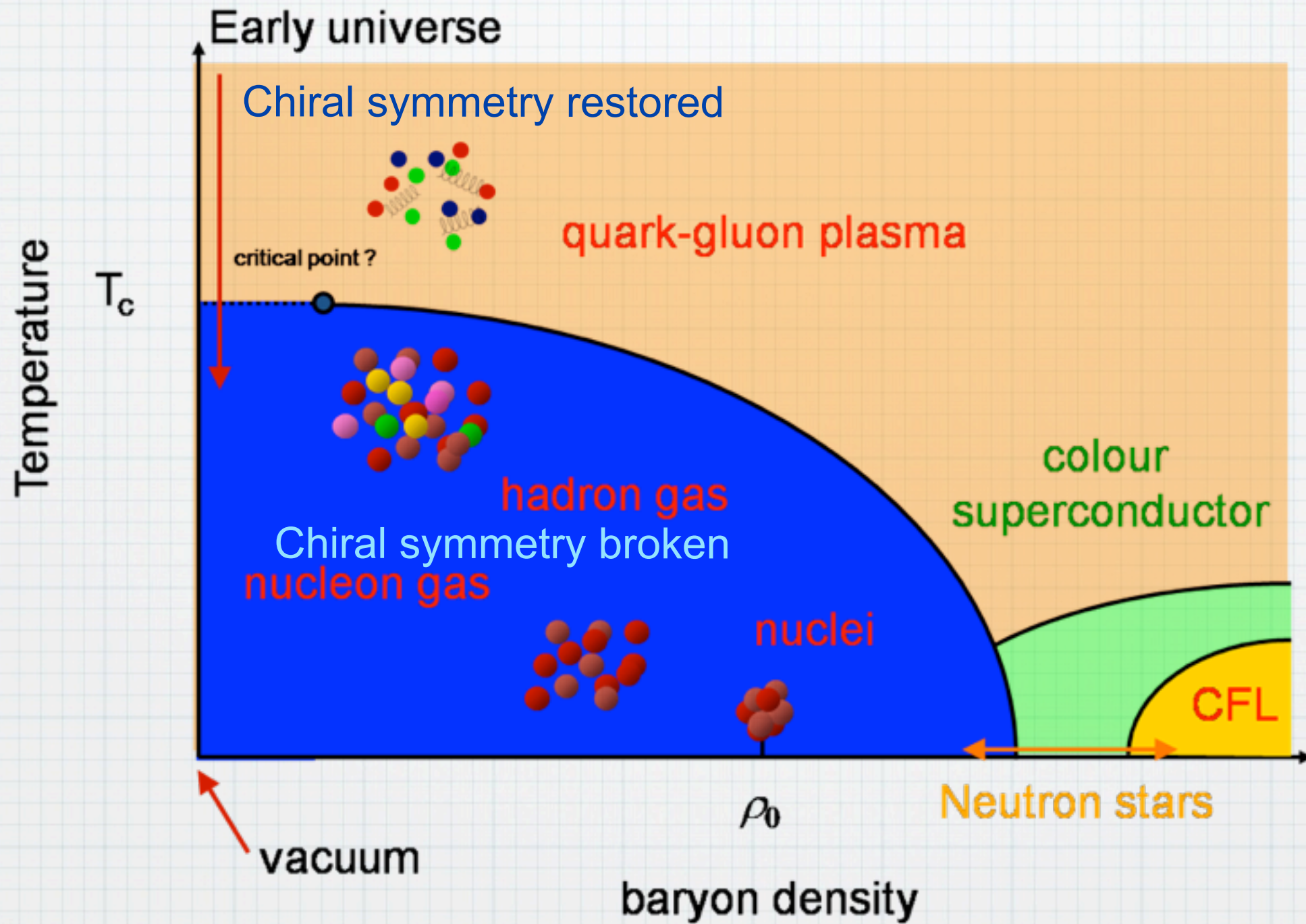


**Chiral Symmetry:** broken

**Chiral Symmetry:** restored

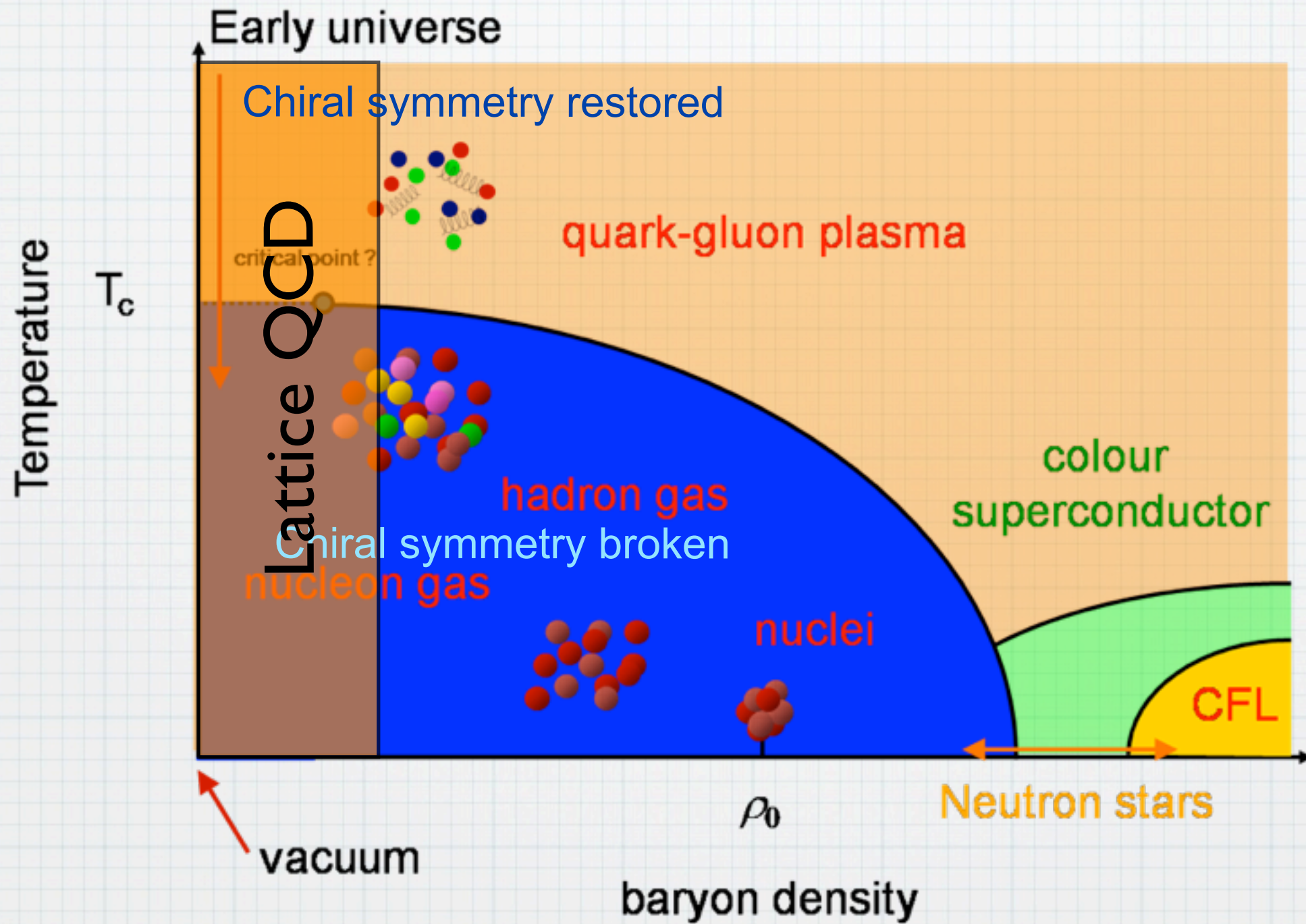


# QCD Phase Diagram



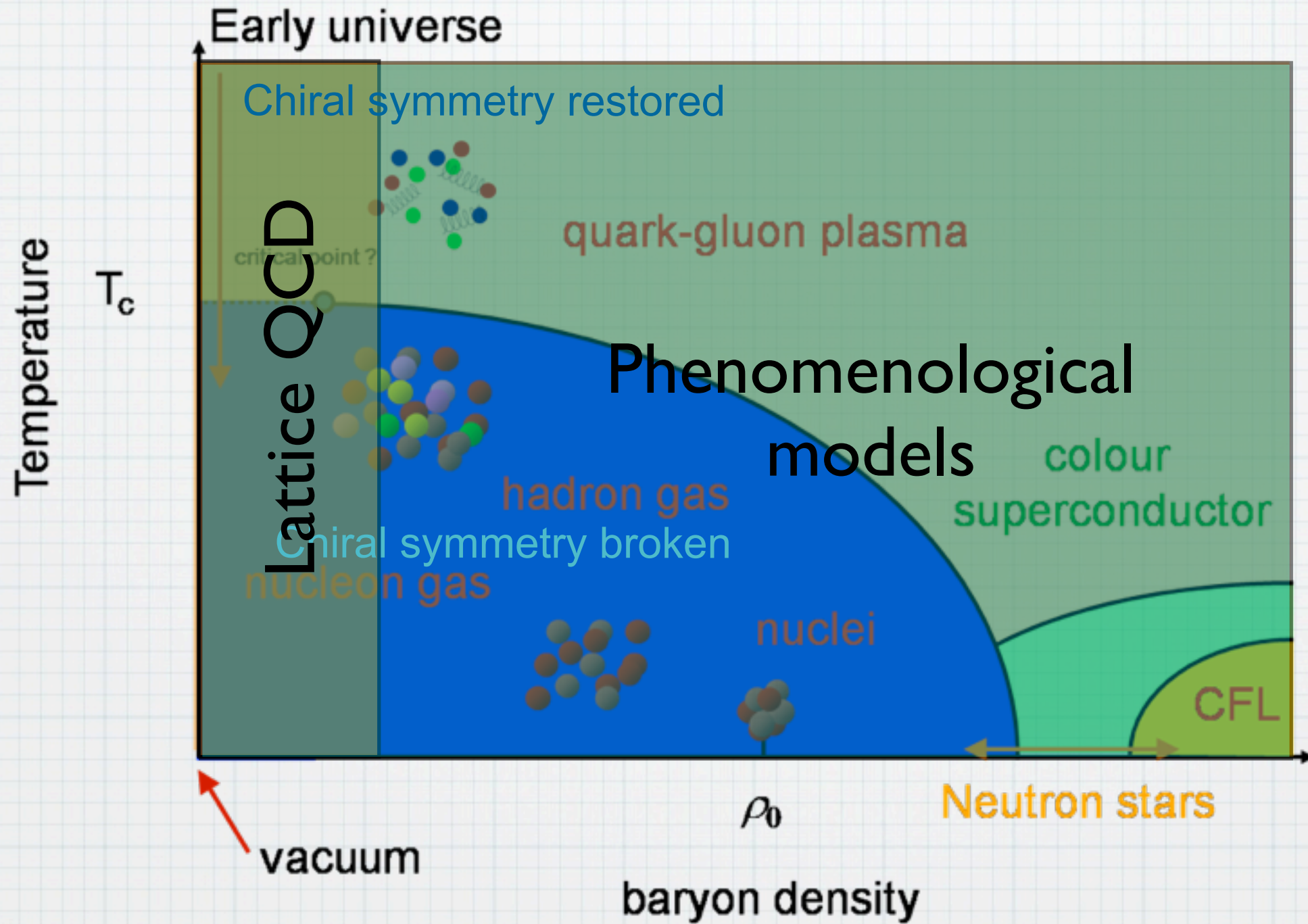


# QCD Phase Diagram





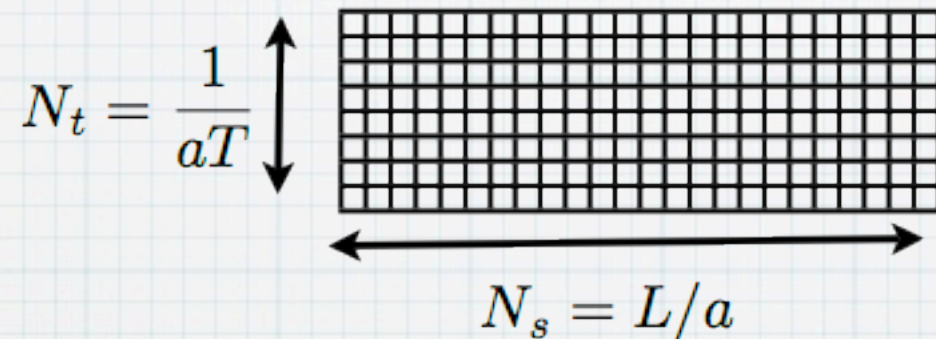
# QCD Phase Diagram





# Lattice QCD

- \* Analytic or perturbative solutions **in low-energy QCD** are hard or impossible due to the **highly nonlinear nature** of the strong force
- \* Lattice QCD: well-established **non-perturbative approach** to solving QCD
- \* Solving QCD on a grid of points in space and time
- \* The lattice action is the parameterization used to discretize the Lagrangian of QCD on a space-time grid



- \* From the partition function  $Z$ , knowledge of all the thermodynamics

$$F = -T \ln Z ,$$
$$p = \frac{\partial(T \ln Z)}{\partial V} ,$$
$$S = \frac{\partial(T \ln Z)}{\partial T} ,$$

$$\bar{N}_i = \frac{\partial(T \ln Z)}{\partial \mu_i} ,$$
$$E = -pV + TS + \mu_i \bar{N}_i$$



# Sign problem

\* The QCD path integral is computed by **Monte Carlo algorithms** which samples field configurations with a weight proportional to the **exponential of the action**

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

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

\* If the action is **complex**, its exponential is **oscillating**: it cannot be used as a probability

\* This is the reason why lattice QCD simulations cannot presently be performed at finite chemical potential

\* Possible solutions:

- ➔ Taylor expansion around  $\mu_B=0$
- ➔ Imaginary chemical potential
- ➔ Reweighting technique

All valid at small chemical potentials



# Phase transitions and order parameters

- \* We want to study the transition **from hadrons to the QGP**: **deconfinement** and **chiral symmetry restoration**
- \* A **phase transition** is the transformation of a thermodynamic system from one phase or state of matter to another
- \* During a phase transition of a given medium **certain properties of the medium change**, often discontinuously, as a result of some **external conditions**
- \* The measurement of the external conditions at which the transformation occurs is called the **phase transition point**
- \* **Order parameter**: some observable physical quantity that is able to **distinguish between two distinct phases**
- \* We need to find observables which allow us to **distinguish** between **confined/deconfined** system and between **chirally broken/restored** phase



# Polyakov loop: deconfinement

\* We consider a system of gluons in which we put a heavy quark-antiquark pair as a probe

$$\langle \Phi \rangle \sim e^{-F/T}$$

→ How much energy  $F$  is needed to extract the heavy quark from the system?

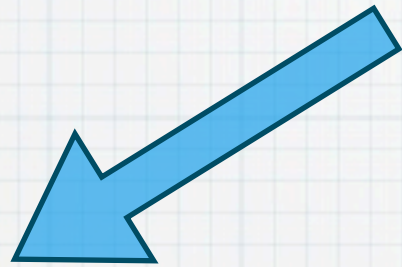


# Polyakov loop: deconfinement

\* We consider a system of gluons in which we put a heavy quark-antiquark pair as a probe

$$\langle \Phi \rangle \sim e^{-F/T}$$

→ How much energy  $F$  is needed to extract the heavy quark from the system?



Confined system  
Infinite energy is  
needed

$$\langle \Phi \rangle = 0$$

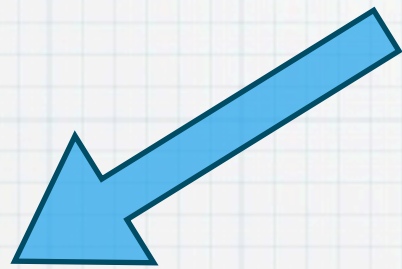


# Polyakov loop: deconfinement

\* We consider a system of gluons in which we put a heavy quark-antiquark pair as a probe

$$\langle \Phi \rangle \sim e^{-F/T}$$

→ How much energy  $F$  is needed to extract the heavy quark from the system?



Confined system  
Infinite energy is  
needed

$$\langle \Phi \rangle = 0$$

Deconfined system  
finite energy is  
needed

$$\langle \Phi \rangle \rightarrow 1$$

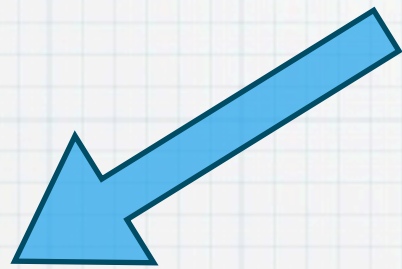


# Polyakov loop: deconfinement

\* We consider a system of gluons in which we put a heavy quark-antiquark pair as a probe

$$\langle \Phi \rangle \sim e^{-F/T}$$

→ How much energy  $F$  is needed to extract the heavy quark from the system?



Confined system  
Infinite energy is  
needed

$$\langle \Phi \rangle = 0$$

Deconfined system  
Finite energy is  
needed

$$\langle \Phi \rangle \rightarrow 1$$

**Polyakov loop: order parameter for deconfinement**

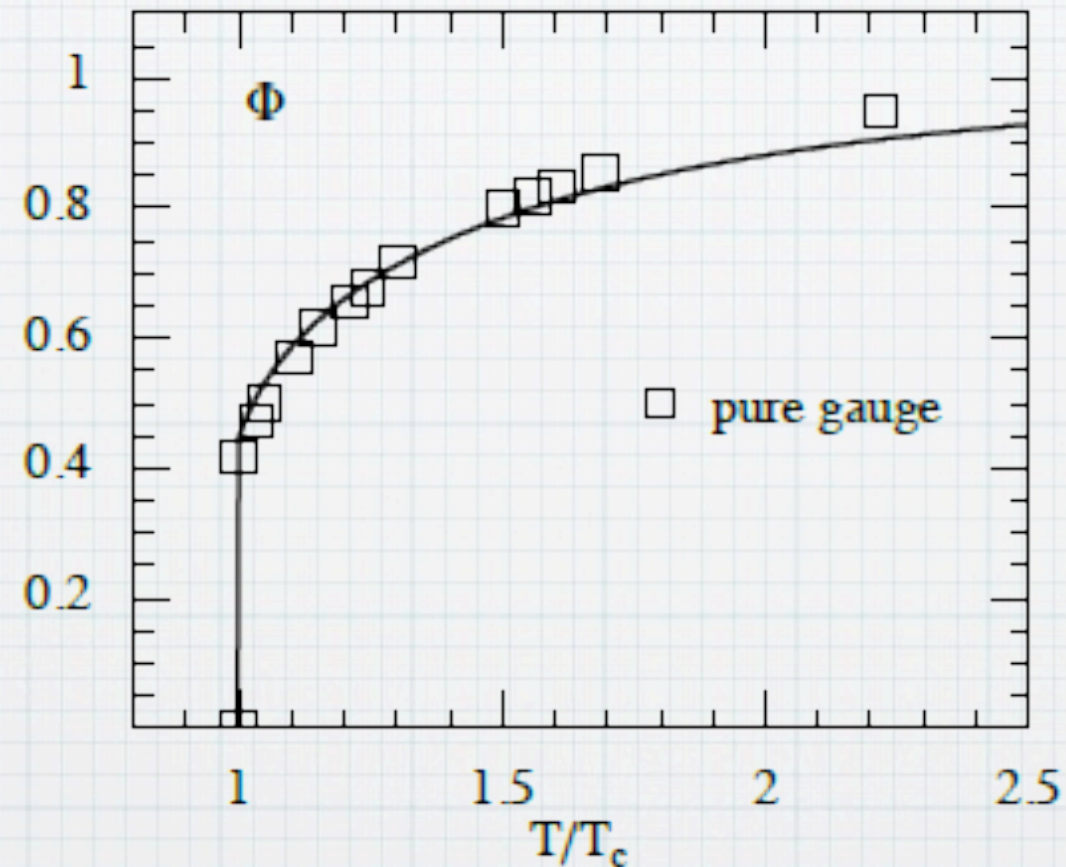


# Polyakov loop: deconfinement

\* We consider a system of gluons in which we put a heavy quark-antiquark pair as a probe

$$\langle \Phi \rangle \sim e^{-F/T}$$

→ How much energy  $F$  is needed to extract the heavy quark from the system?



**Polyakov loop: order parameter for deconfinement**

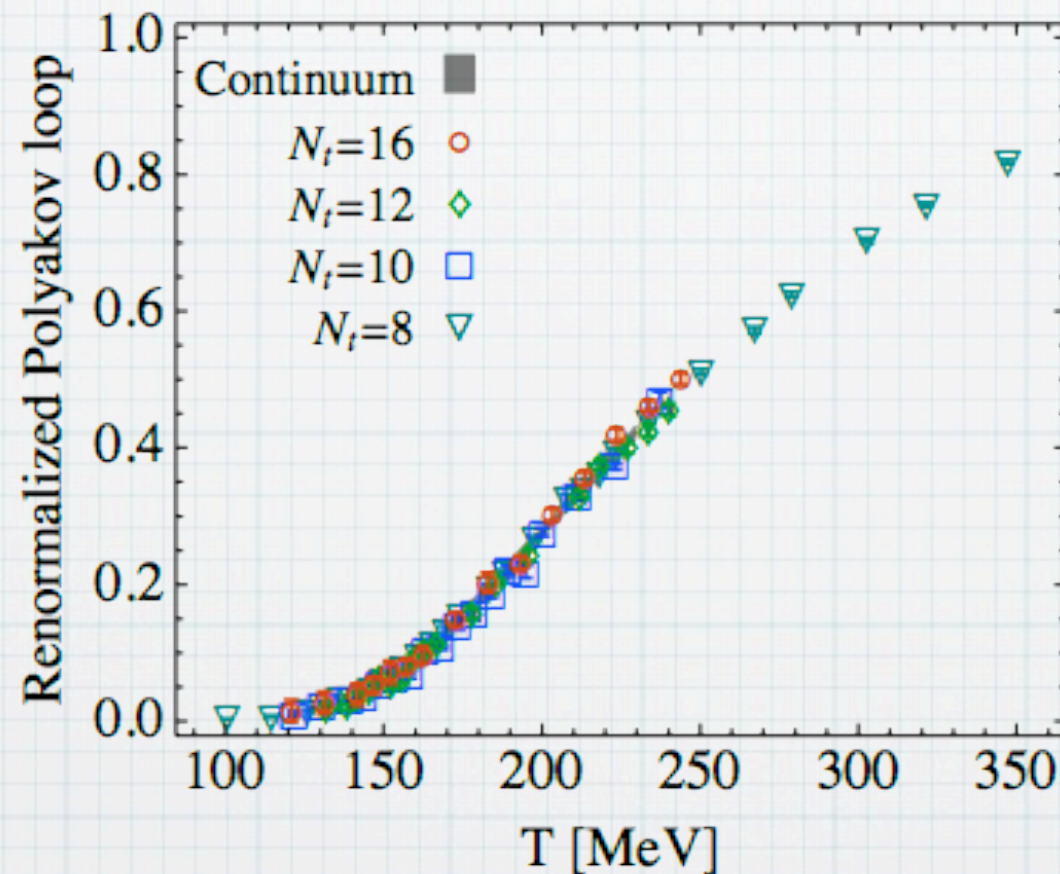


# Polyakov loop: deconfinement

\* We consider a system of gluons in which we put a heavy quark-antiquark pair as a probe

$$\langle \Phi \rangle \sim e^{-F/T}$$

→ How much energy  $F$  is needed to extract the heavy quark from the system?



For QCD with physical quark masses the transition is a smooth crossover

**Polyakov loop: order parameter for deconfinement**

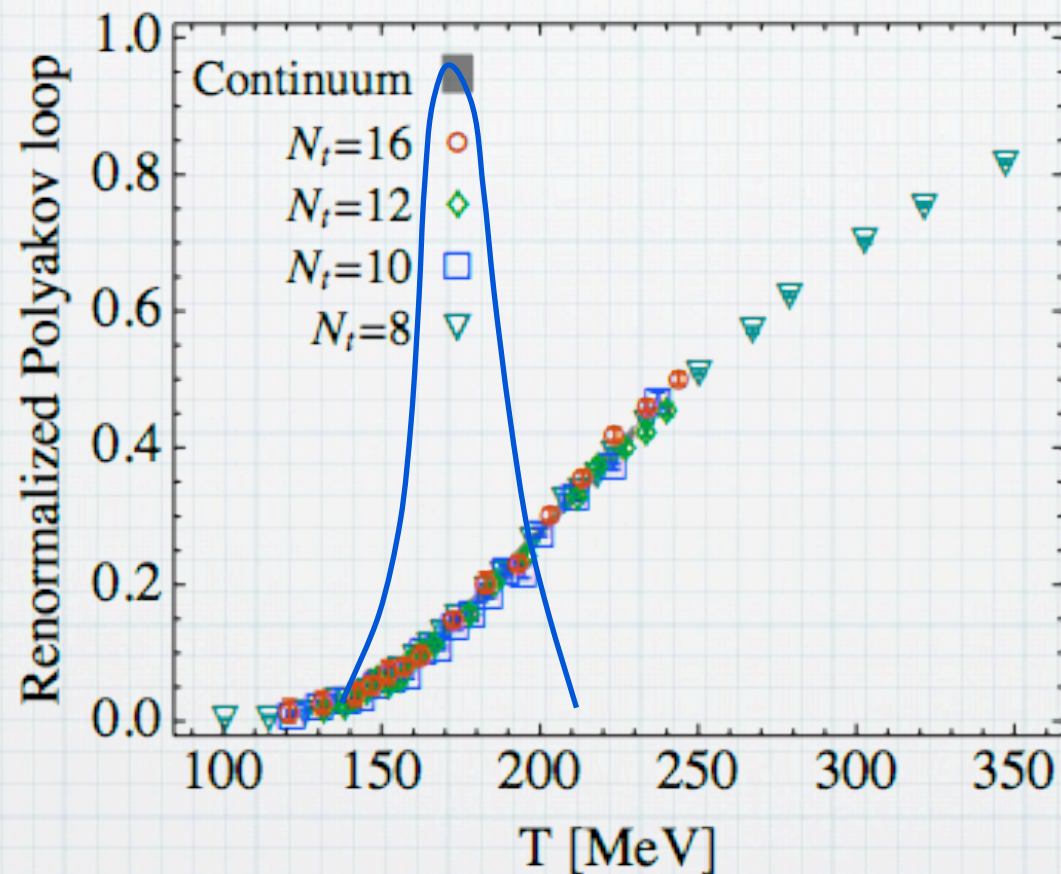


# Polyakov loop: deconfinement

\* We consider a system of gluons in which we put a heavy quark-antiquark pair as a probe

$$\langle \Phi \rangle \sim e^{-F/T}$$

→ How much energy  $F$  is needed to extract the heavy quark from the system?



For QCD with physical quark masses the transition is a smooth crossover

**Polyakov loop: order parameter for deconfinement**



# Chiral condensate: chiral transition

- \* The chiral condensate  $\langle \bar{\psi}\psi \rangle$  is the vacuum expectation value of the operator  $\bar{\psi}\psi$ .
- \* The magnitude of the constituent quark mass is proportional to it
  - Even if the “bare” quark mass in the QCD Lagrangian is small, they develop a constituent one, through interaction with the chiral condensate

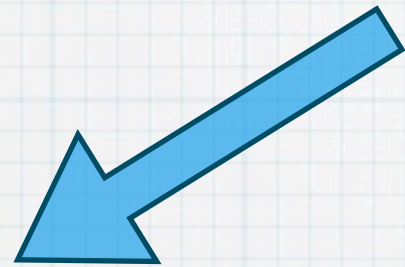


# Chiral condensate: chiral transition

\* The chiral condensate  $\langle \bar{\psi}\psi \rangle$  is the vacuum expectation value of the operator  $\bar{\psi}\psi$ .

\* The magnitude of the constituent quark mass is proportional to it

→ Even if the “bare” quark mass in the QCD Lagrangian is small, they develop a constituent one, through interaction with the chiral condensate



Chirally broken system  
Large effective quark  
mass

$$\langle \bar{\psi}\psi \rangle \neq 0$$

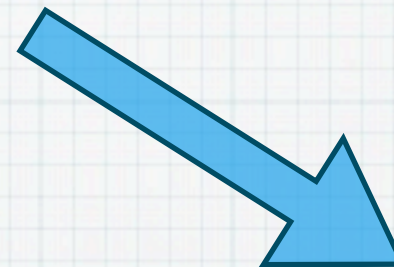
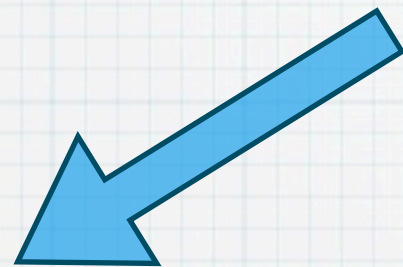


# Chiral condensate: chiral transition

\* The chiral condensate  $\langle \bar{\psi}\psi \rangle$  is the vacuum expectation value of the operator  $\bar{\psi}\psi$ .

\* The magnitude of the constituent quark mass is proportional to it

→ Even if the “bare” quark mass in the QCD Lagrangian is small, they develop a constituent one, through interaction with the chiral condensate



Chirally broken system  
Large effective quark  
mass

$$\langle \bar{\psi}\psi \rangle \neq 0$$

Chirally restored system  
Small effective quark  
mass

$$\langle \bar{\psi}\psi \rangle = 0$$

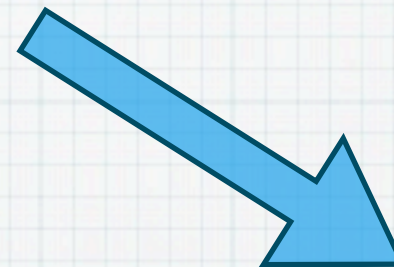
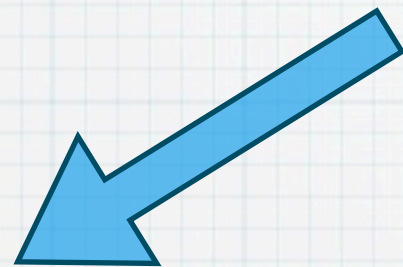


# Chiral condensate: chiral transition

\* The chiral condensate  $\langle \bar{\psi}\psi \rangle$  is the vacuum expectation value of the operator  $\bar{\psi}\psi$ .

\* The magnitude of the constituent quark mass is proportional to it

→ Even if the “bare” quark mass in the QCD Lagrangian is small, they develop a constituent one, through interaction with the chiral condensate



Chirally broken system  
Large effective quark  
mass

$$\langle \bar{\psi}\psi \rangle \neq 0$$

Chirally restored system  
Small effective quark  
mass

$$\langle \bar{\psi}\psi \rangle = 0$$

**Chiral condensate: order parameter for  
chiral phase transition**

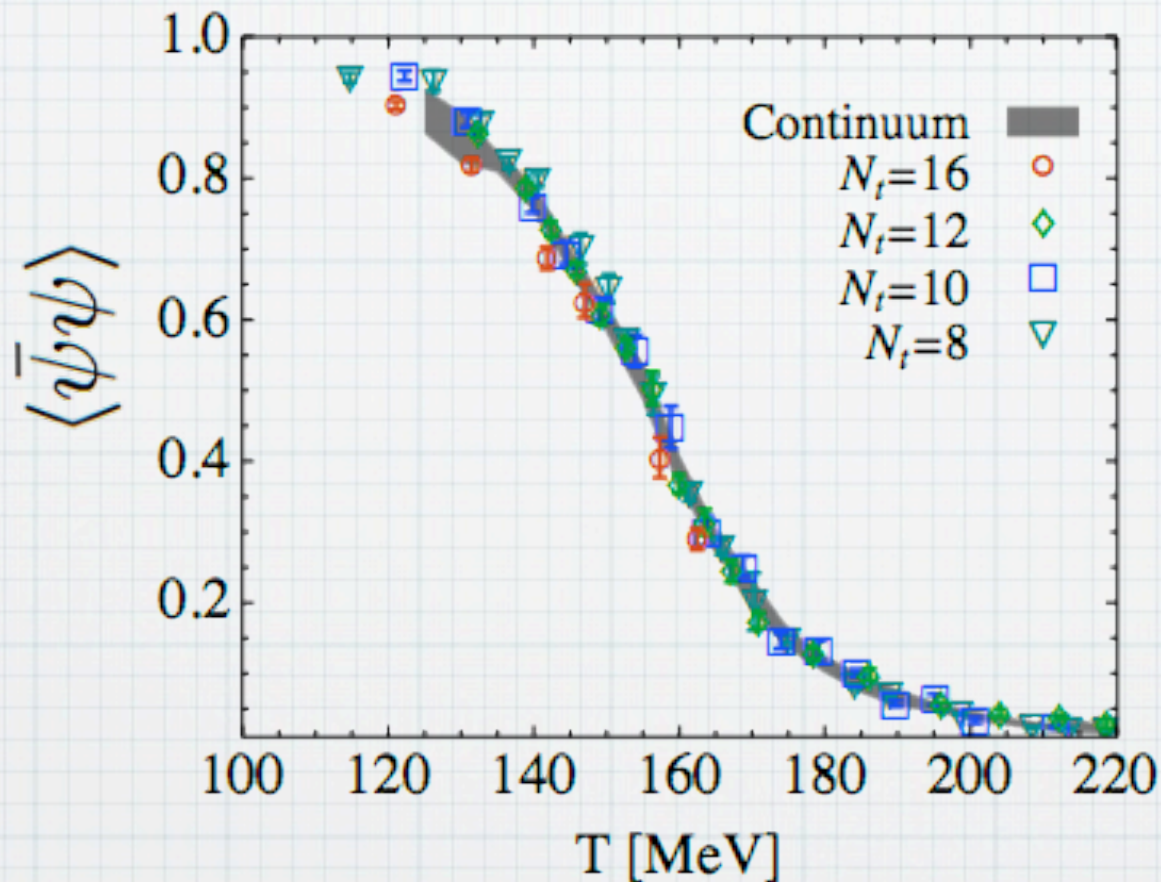


# Chiral condensate: chiral transition

\* The chiral condensate  $\langle \bar{\psi}\psi \rangle$  is the vacuum expectation value of the operator  $\bar{\psi}\psi$ .

\* The magnitude of the constituent quark mass is proportional to it

→ Even if the “bare” quark mass in the QCD Lagrangian is small, they develop a constituent one, through interaction with the chiral condensate



For QCD with physical quark masses the transition is a smooth crossover

**Chiral condensate: order parameter for chiral phase transition**

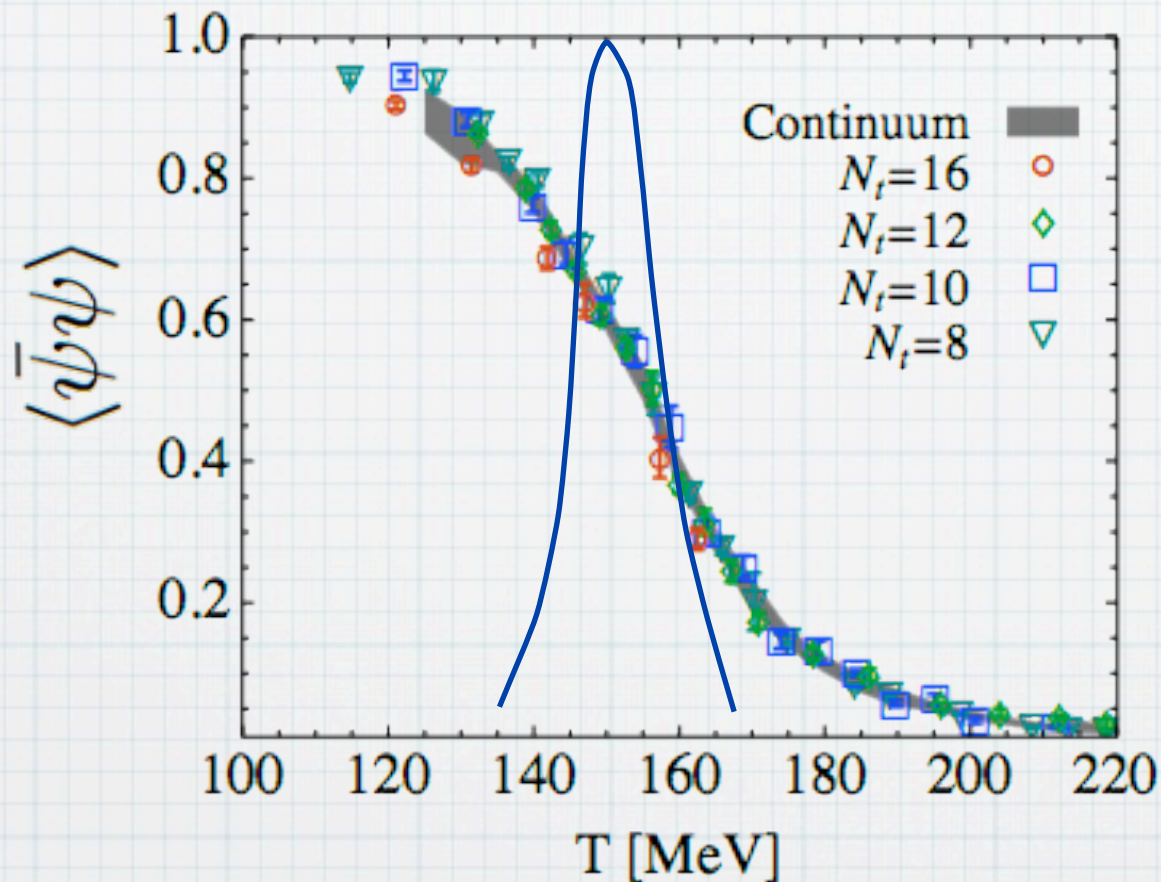


# Chiral condensate: chiral transition

\* The chiral condensate  $\langle \bar{\psi}\psi \rangle$  is the vacuum expectation value of the operator  $\bar{\psi}\psi$ .

\* The magnitude of the constituent quark mass is proportional to it

➔ Even if the “bare” quark mass in the QCD Lagrangian is small, they develop a constituent one, through interaction with the chiral condensate

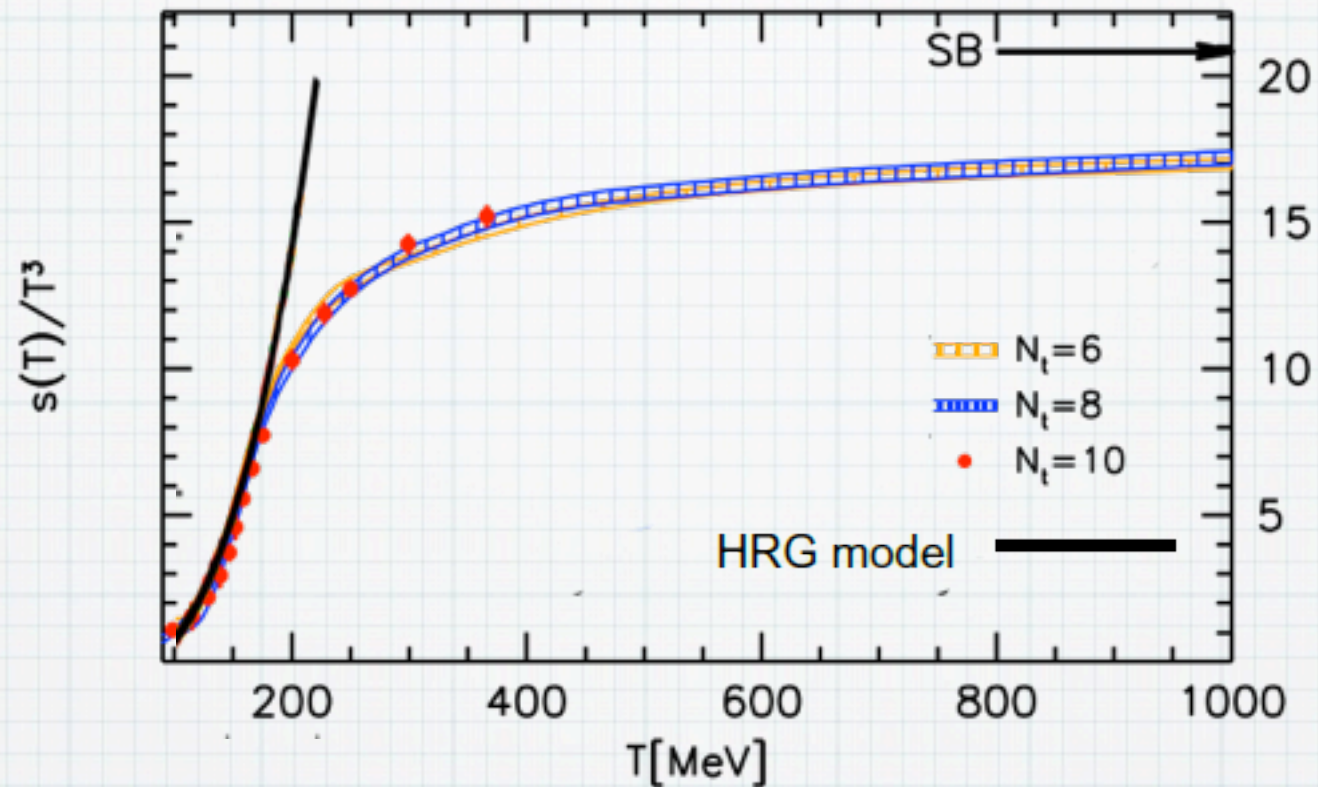


For QCD with physical quark masses the transition is a smooth crossover

**Chiral condensate: order parameter for chiral phase transition**



# Transition from QCD Thermodynamics



\*  $s/T^3$  indicates the number of particle species

\* Rapid rise = liberation of degrees of freedom

\* Compare to an ideal gas of quarks and gluons

$$s = \frac{4g}{\pi^2} T^3$$

\* This gives us an idea of how strong is the interaction



# What happens below $T_c$ ?

\* At low  $T$  and  $\mu_B=0$ , QCD thermodynamics is dominated by **pions**

\* as  $T$  increases, heavier hadrons start to contribute

\* Their mutual interaction is suppressed:

$$n_i n_k \sim \exp[-(M_i + M_k)/T]$$

\* **Interacting** hadronic matter in the ground state can be well approximated by a **non-interacting** gas of **hadronic resonances**

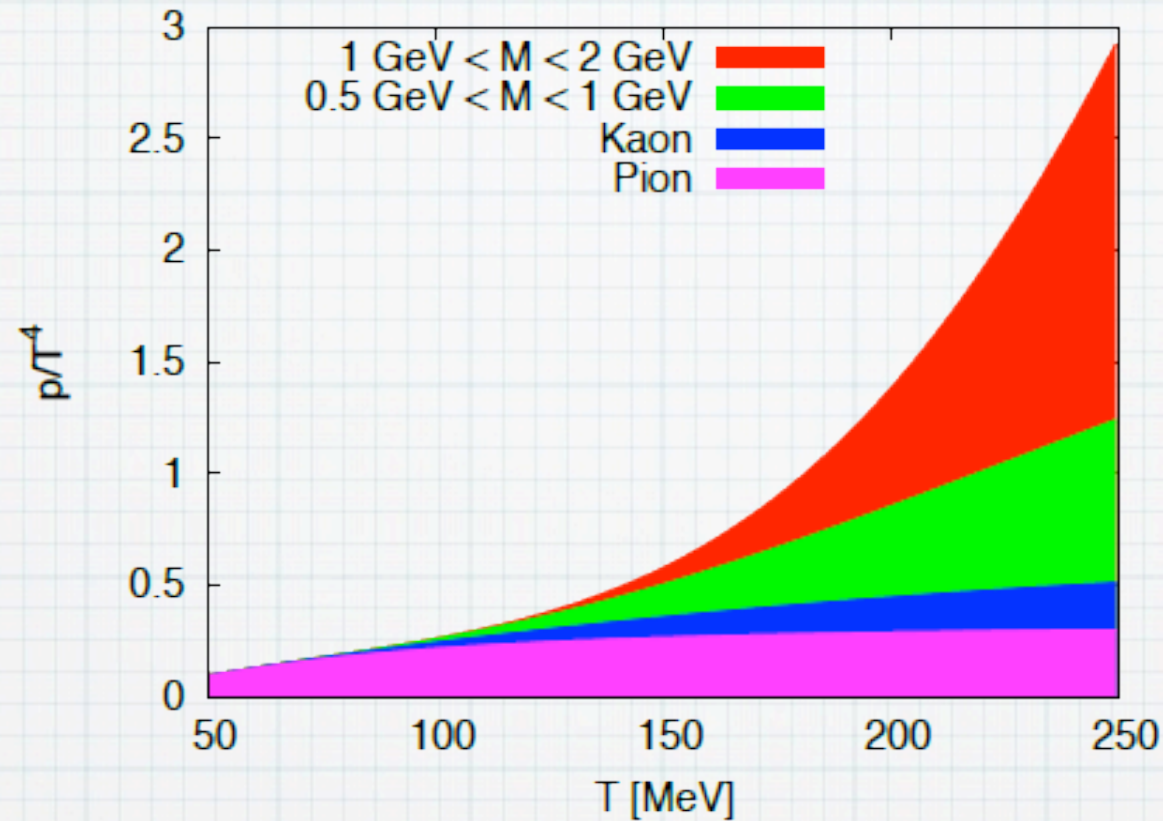
$$p^{HRG}/T^4 = \frac{1}{VT^3} \sum_{i \in \text{mesons}} \ln Z_{m_i}^M(T, V, \mu_{X^a}) + \frac{1}{VT^3} \sum_{i \in \text{baryons}} \ln Z_{m_i}^B(T, V, \mu_{X^a}),$$

with  $\ln Z_{m_i}^{M/B} = \mp \frac{V d_i}{2\pi^2} \int_0^\infty dk k^2 \ln(1 \mp z_i e^{-\epsilon_i/T})$ ,  $\epsilon_i = \sqrt{k^2 + m_i^2}$ ,

$z_i = \exp\left(\frac{\sum_a X_i^a \mu_{X^a}}{T}\right)$  and  $X^a$  are all conserved charges.



# How many resonances do we include?



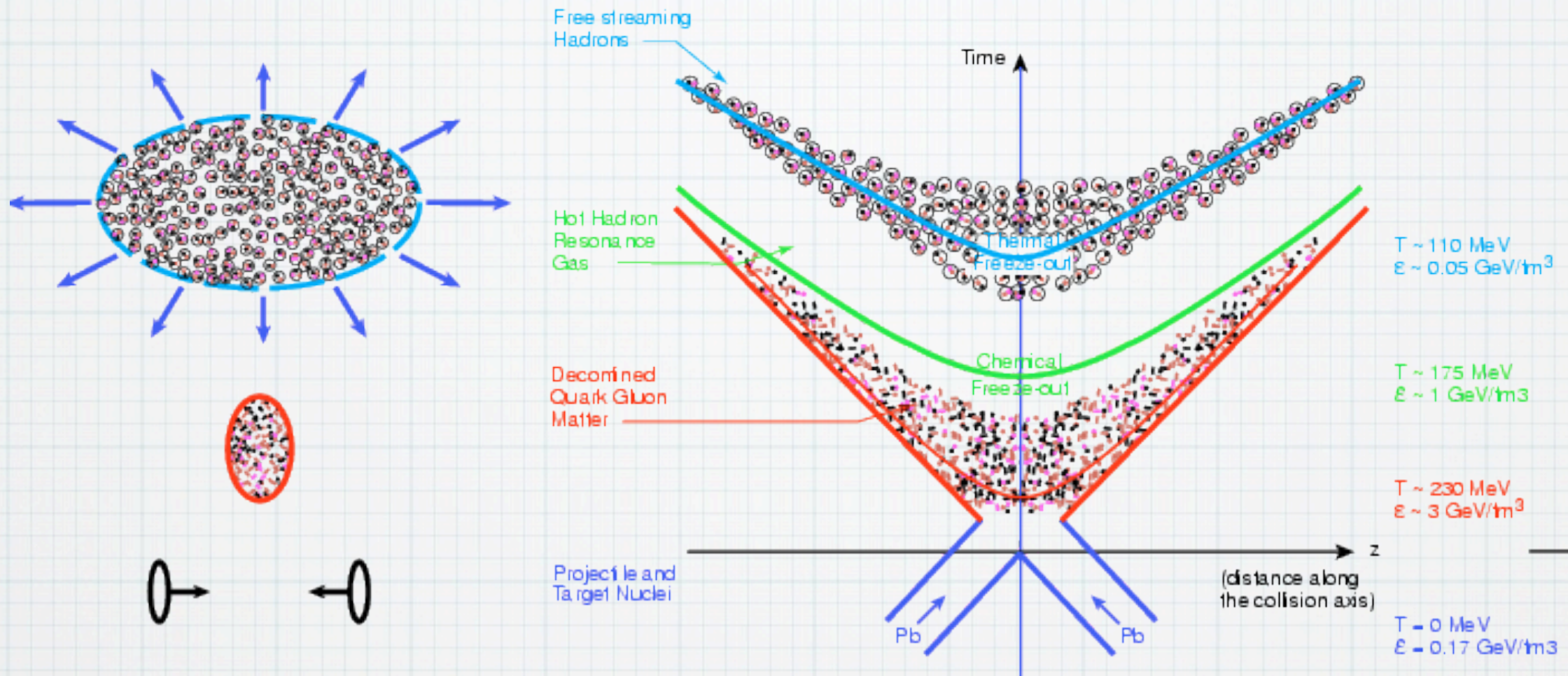
\* With different mass cut-offs we can separate the contribution of different particles

\* Known resonances up to  $M=2.5 \text{ GeV}$

\*  $\sim 170$  different masses  $\longleftrightarrow$  **1500 resonances**



# Evolution of a heavy-ion collision



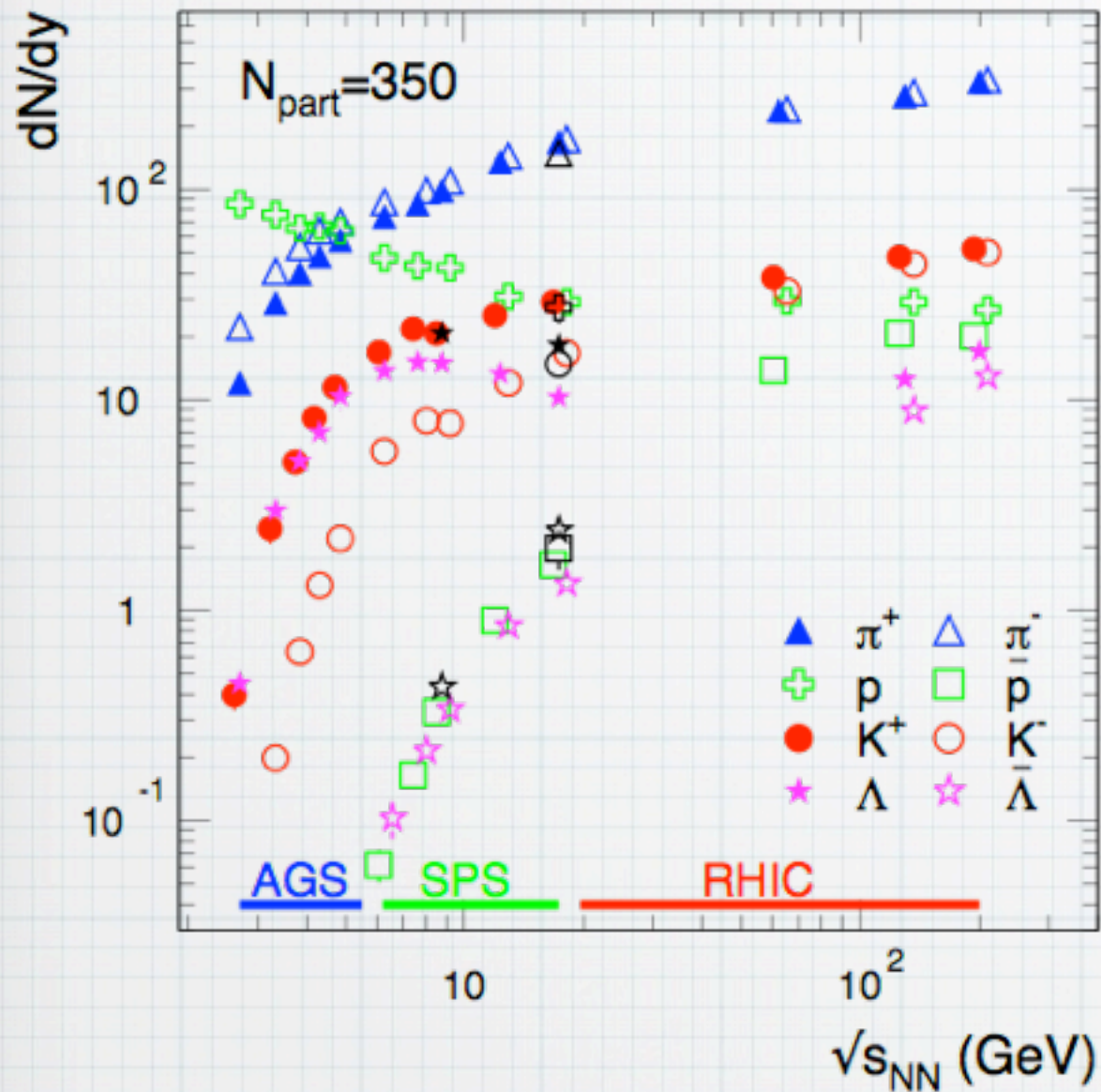
\* **Chemical freeze-out:** inelastic reactions cease: the chemical composition of the system is fixed (particle yields and fluctuations)

\* **Kinetic freeze-out:** elastic reactions cease: spectra and correlations are frozen (free streaming of hadrons)

\* Hadrons reach the detector



# Hadron yields



\*  $E=mc^2$ : lots of particles are created

\* Particle counting (average over many events)

\* Take into account:

\* detector inefficiency

\* missing particles at low  $p_T$

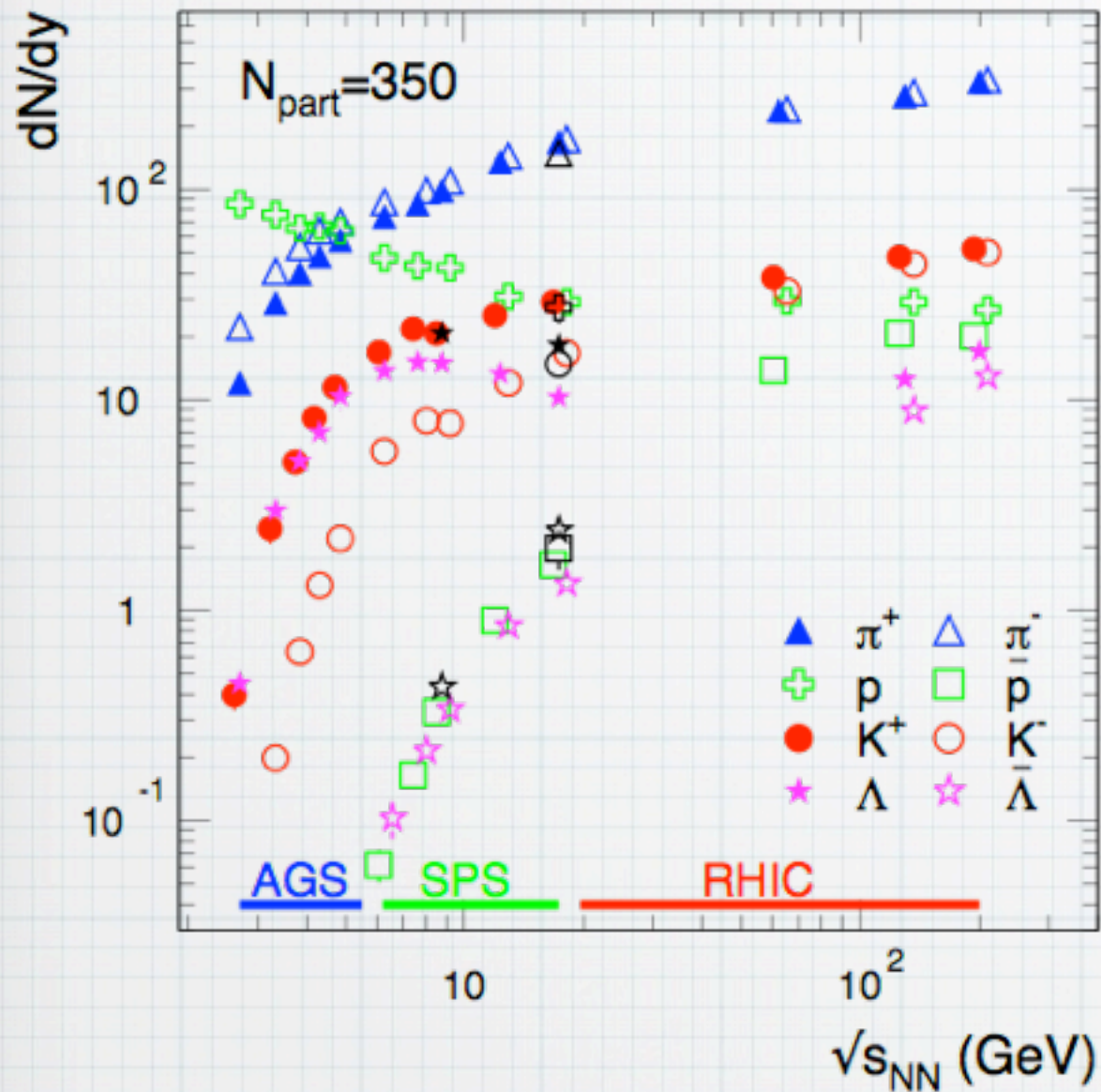
\* decays

\* HRG model: test hypothesis of hadron abundancies in equilibrium

$$N_i = -T \frac{\partial \ln Z_i}{\partial \mu} = \frac{g_i V}{2\pi^2} \int_0^\infty \frac{p^2 dp}{\exp[(E_i - \mu_i)/T] \pm 1}$$



# Hadron yields



\*  $E=mc^2$ : lots of particles are created

\* Particle counting (average over many events)

\* Take into account:

\* detector inefficiency

\* missing particles at low  $p_T$

\* decays

\* HRG model: test hypothesis of hadron abundancies in equilibrium

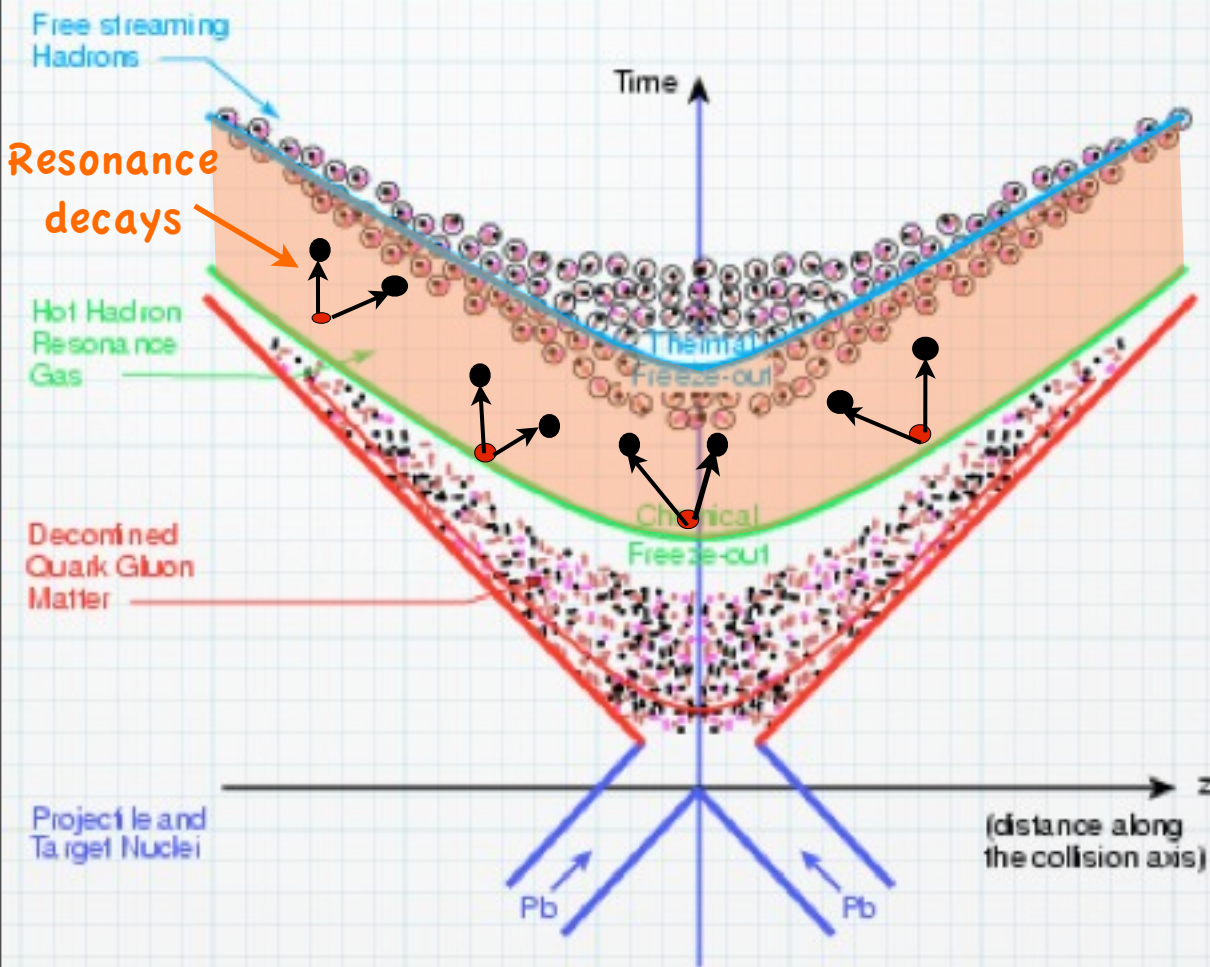
\* We need:

\* a complete hadron spectrum

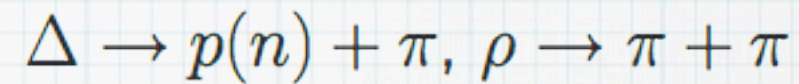
\* control the hadron fraction from decays



# Decays

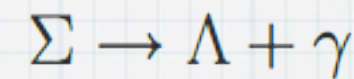


\* All hadrons are subject to **strong and electromagnetic decays**

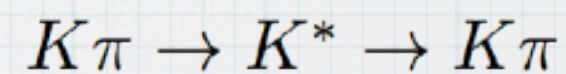
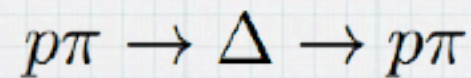
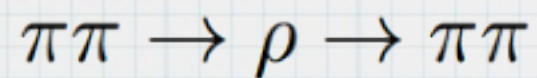


\* e.g. pions: **1/4** primordial, **3/4** from strong decays

\* Weak decays can be treated too:



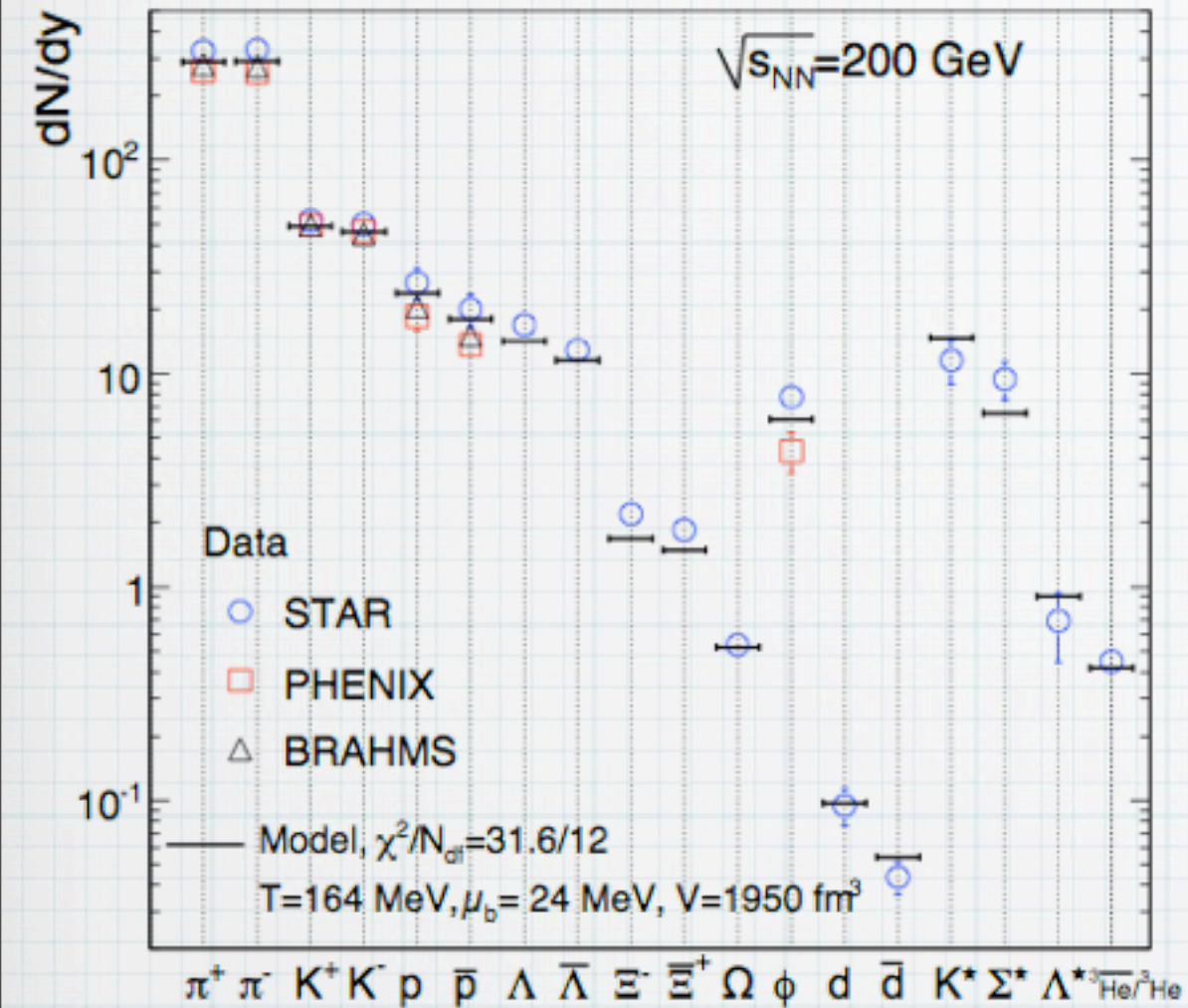
\* **after chemical freeze-out:** only elastic and quasi-elastic scatterings take place:



$$\bar{N}_i = N_i + \sum_r d_{r \rightarrow i} N_r$$



# The thermal fits

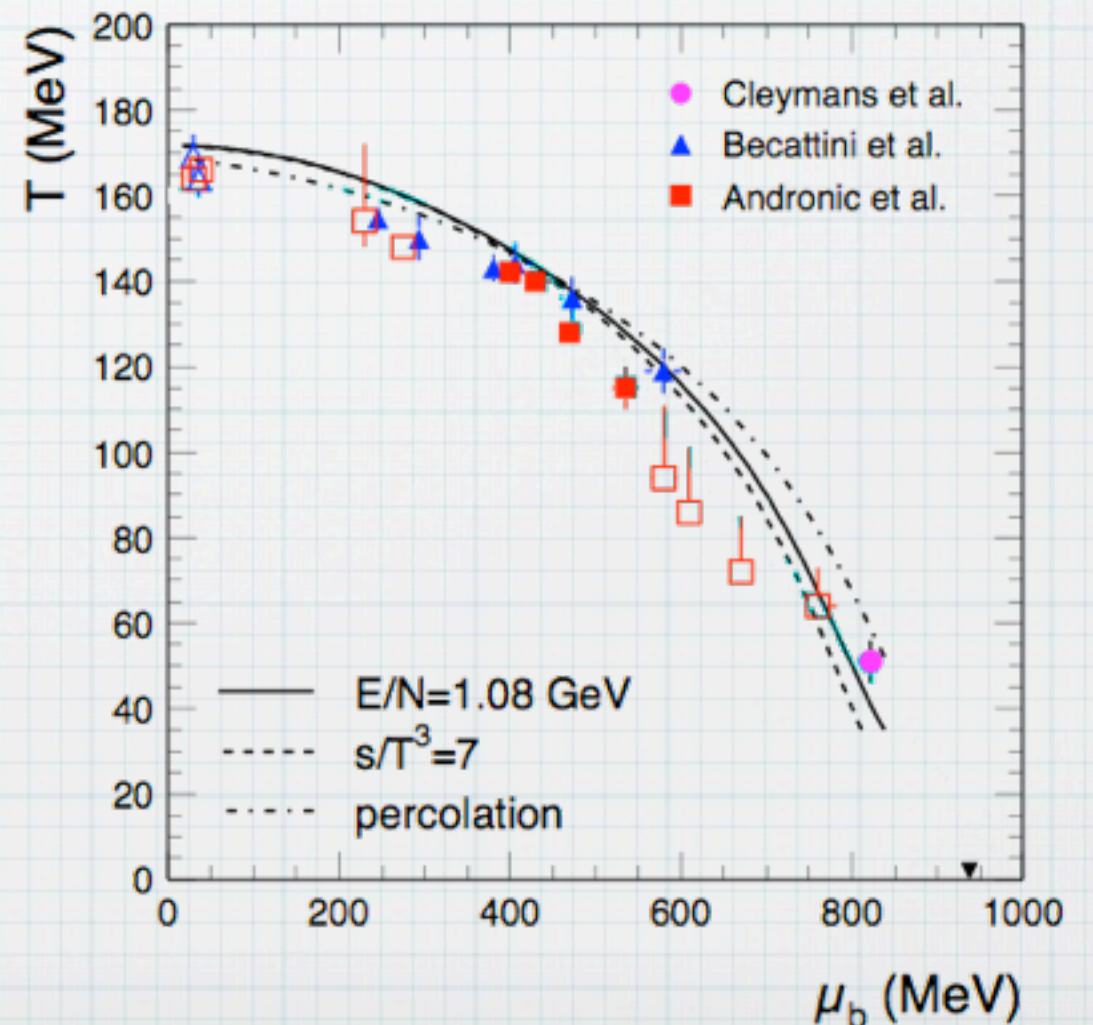


\* Fit is performed minimizing the  $\chi^2$

\* **Fit to yields:** parameters  $T, \mu_B, V$

\* **Fit to ratios:** the volume  $V$  cancels out

\* Changing the collision energy, it is possible to draw the freeze-out line in the  $T, \mu_B$  plane





# Caveats

- \* These results are model-dependent
  - \* they depend on the **particle spectrum** which is included in the model
  - \* possibility of having heavier states with **exponential mass spectrum**
  - \* not known experimentally but can be postulated
  - \* their decay modes are not known



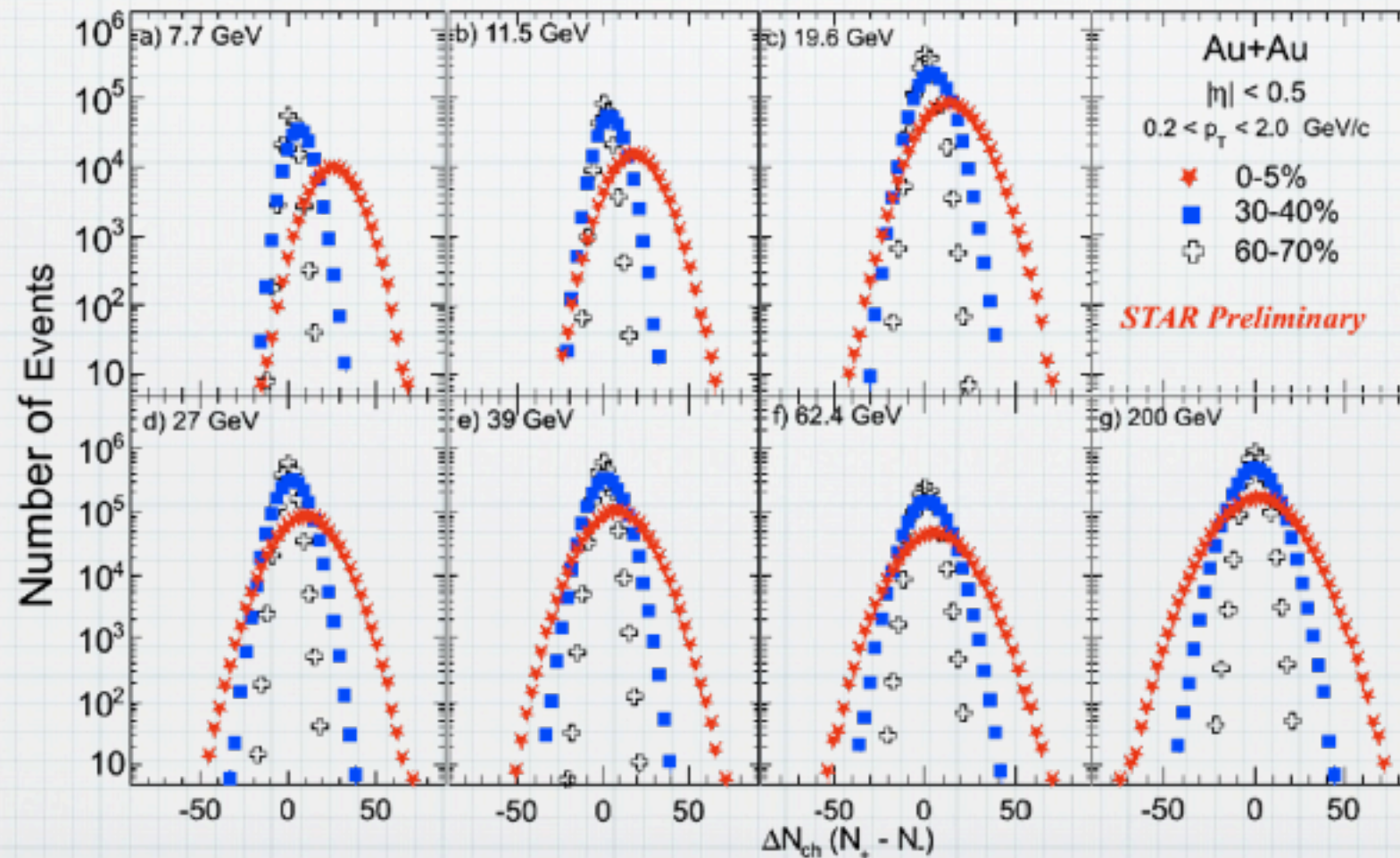
# Caveats

- \* These results are model-dependent
  - \* they depend on the **particle spectrum** which is included in the model
  - \* possibility of having heavier states with **exponential mass spectrum**
  - \* not known experimentally but can be postulated
  - \* their decay modes are not known
- \* Purpose: extract freeze-out parameters **from first principles**
  - \* direct comparison between **experimental measurement** and **lattice QCD results**
  - \* observable: fluctuations of conserved charges (electric charge, baryon number and strangeness)
  - \* directly related to moments of multiplicity distribution (measured)
  - \* lattice QCD looks at conserved charges rather than identified particles



# Fluctuations of conserved charges

- \* Consider the number of electrically charged particles  $N_Q$
- \* Its average value over the whole ensemble of events is  $\langle N_Q \rangle$
- \* In experiments it is possible to **measure its event-by-event distribution**

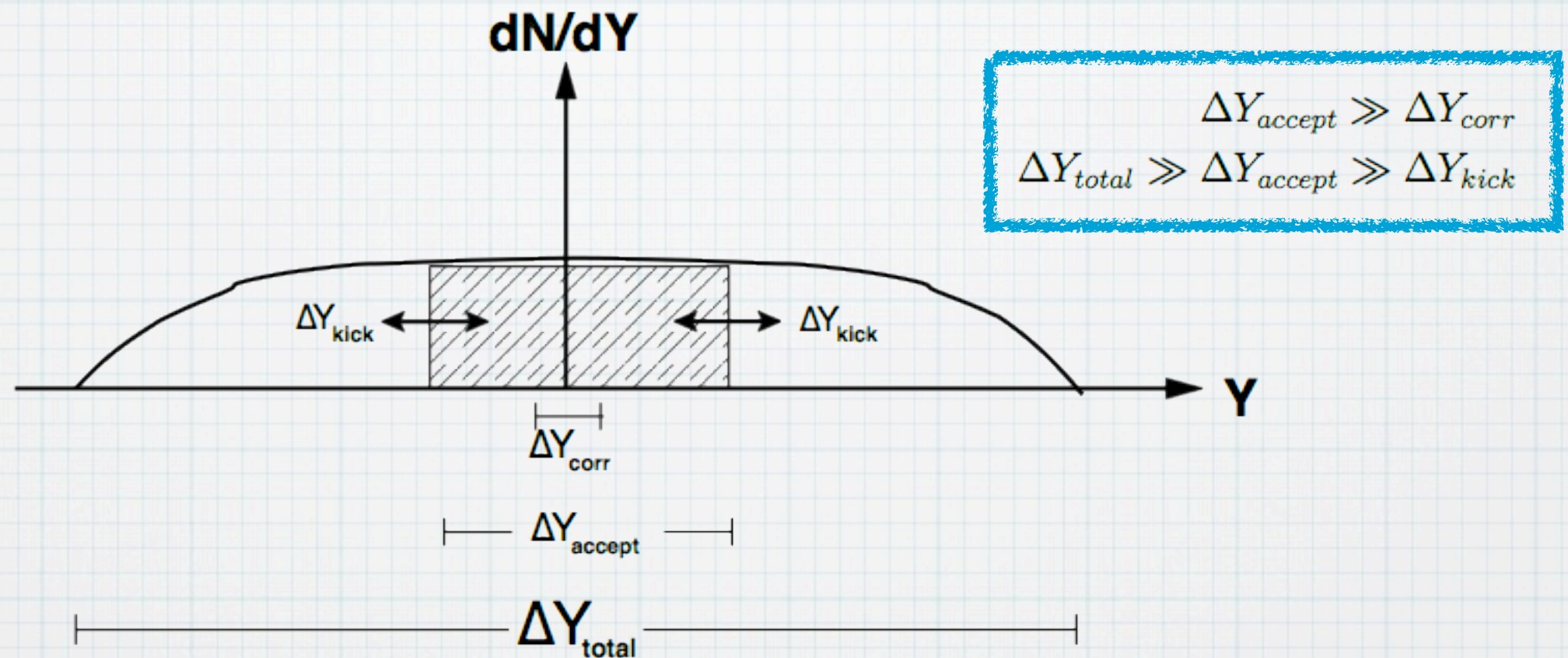




# Fluctuations of conserved charges???

\* If we look at the **entire system**, **none of the conserved charges will fluctuate**

\* By studying a sufficiently **small subsystem**, the fluctuations of conserved quantities become meaningful



➔  $\Delta Y_{total}$ : range for total charge multiplicity distribution

➔  $\Delta Y_{accept}$ : interval for the accepted charged particles

➔  $\Delta Y_{corr}$ : charge correlation length characteristic to the physics of interest

➔  $\Delta Y_{kick}$ : rapidity shift that charges receive during and after hadronization



# Cumulants of multiplicity distribution

\* Deviation of  $N_Q$  from its mean in a single event:  $\delta N_Q = N_Q - \langle N_Q \rangle$

\* The cumulants of the event-by-event distribution of  $N_Q$  are:

$$K_2 = \langle (\delta N_Q)^2 \rangle$$

$$K_3 = \langle (\delta N_Q)^3 \rangle$$

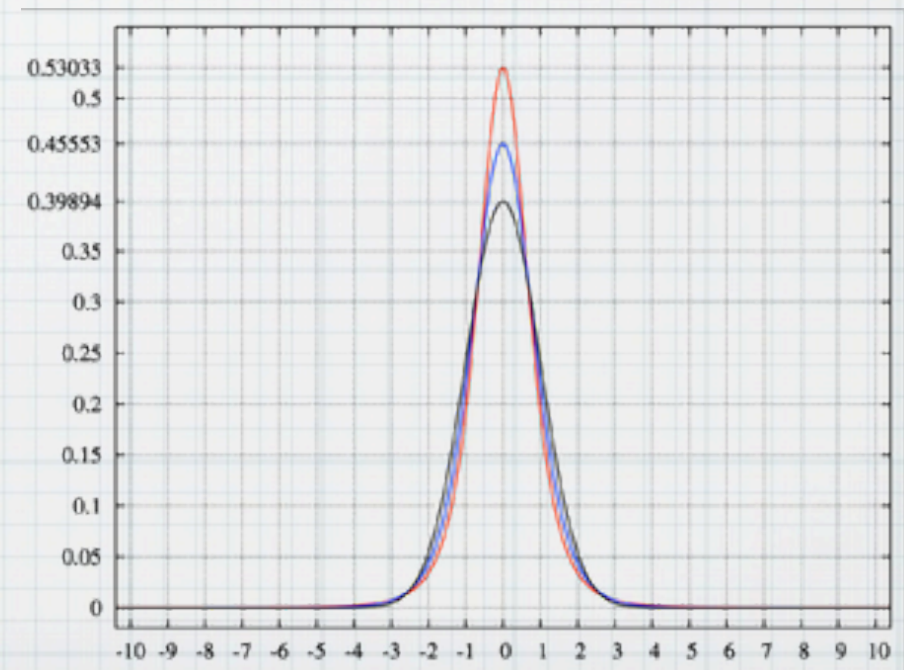
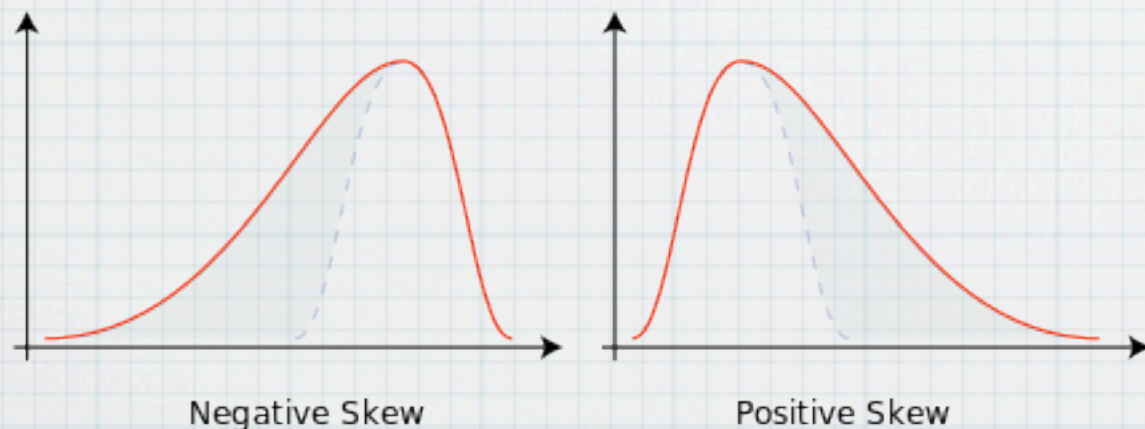
$$K_4 = \langle (\delta N_Q)^4 \rangle - 3 \langle (\delta N_Q)^2 \rangle^2$$

\* The cumulants are related to the central moments of the distribution by:

variance:  $\sigma^2 = K_2$

Skewness:  $S = K_3 / (K_2)^{3/2}$

Kurtosis:  $\kappa = K_4 / (K_2)^2$





# Experimental measurement

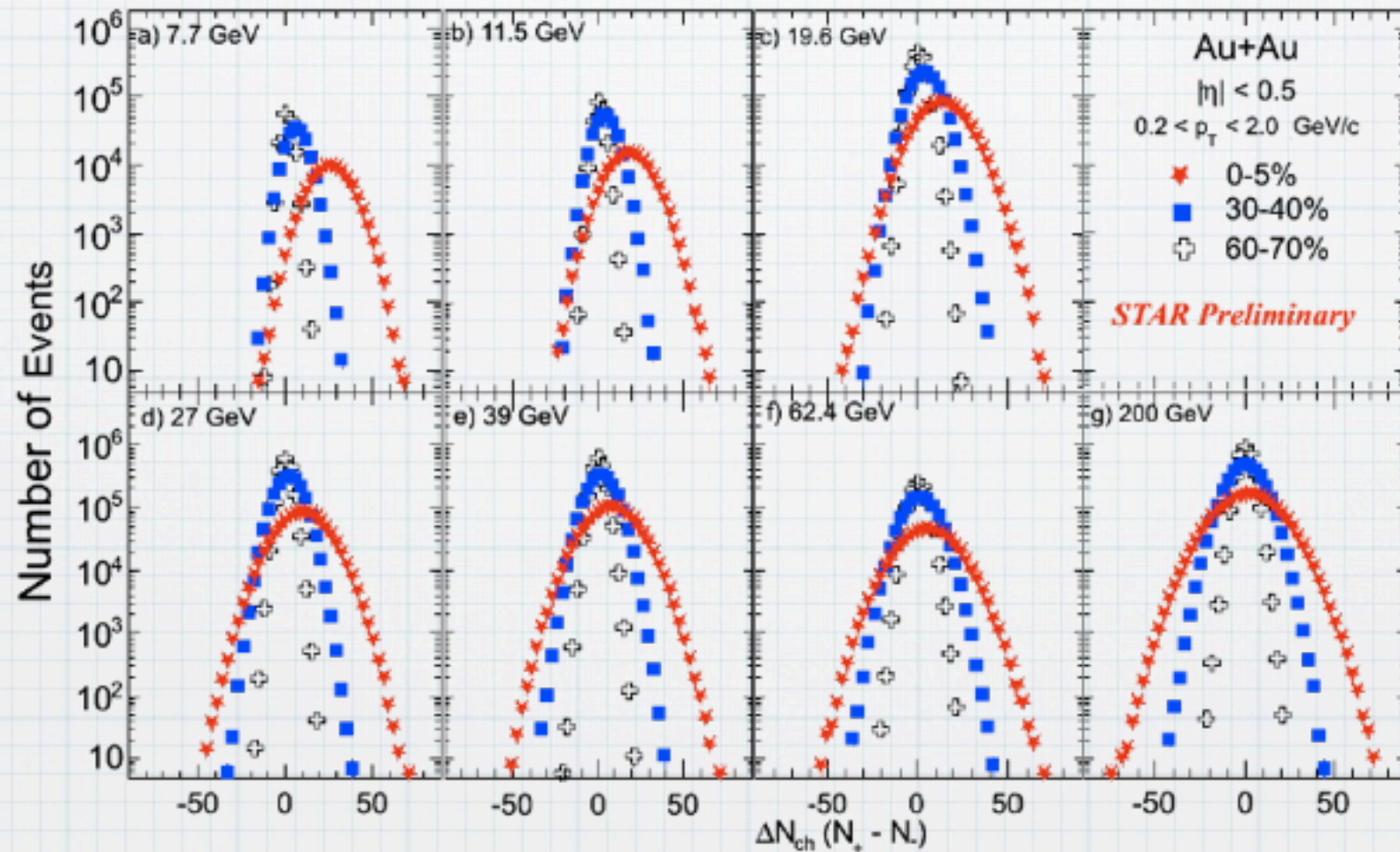
\* Volume-independent ratios:

$$M/\sigma^2 = K_1/K_2$$

$$S\sigma = K_3/K_2$$

$$K\sigma^2 = K_4/K_2$$

$$S\sigma^3/M = K_3/K_1$$





# Experimental measurement

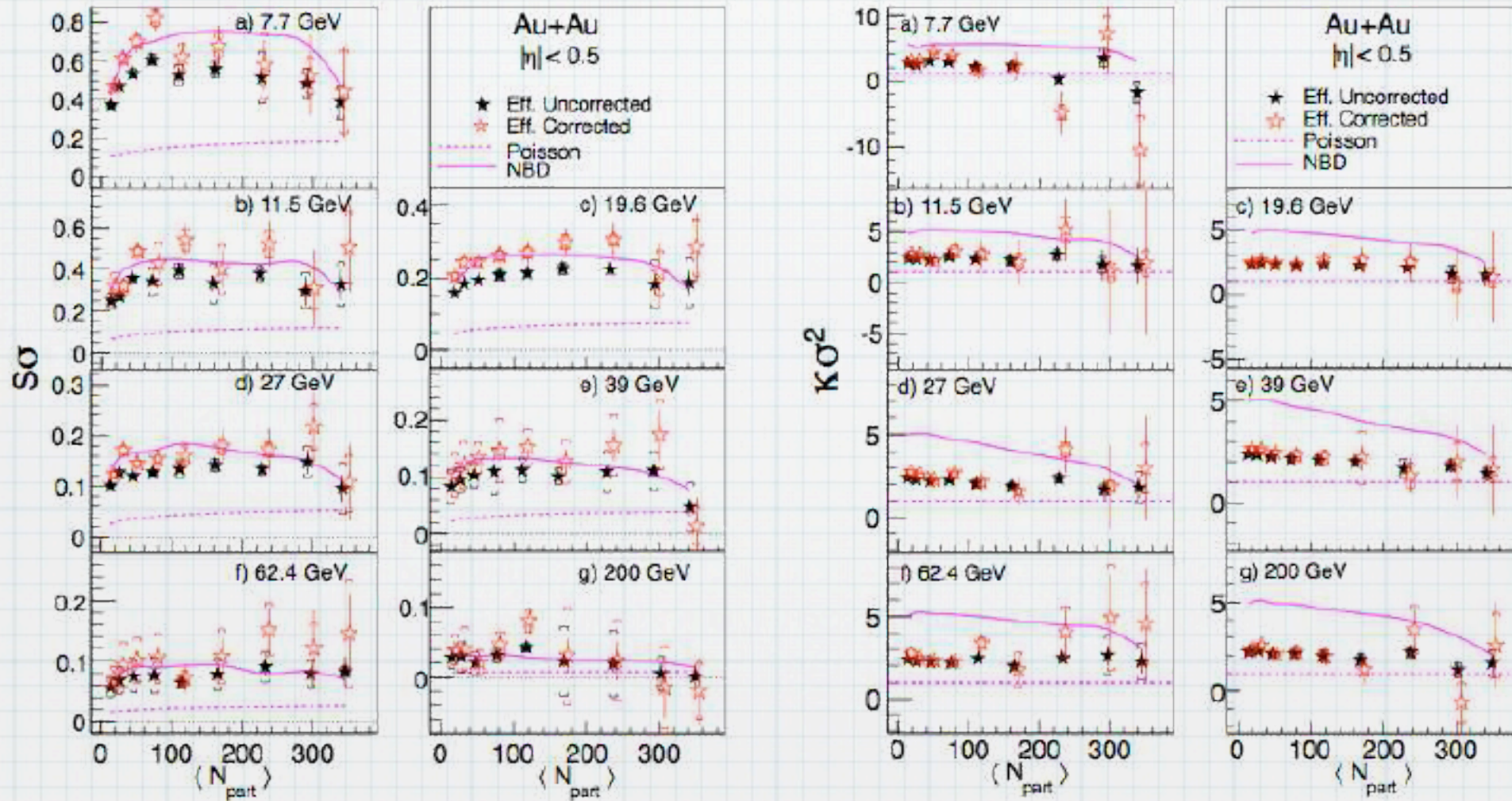
\* Volume-independent ratios:

$$M/\sigma^2 = K_1/K_2$$

$$S\sigma = K_3/K_2$$

$$K\sigma^2 = K_4/K_2$$

$$S\sigma^3/M = K_3/K_1$$





# Susceptibilities of conserved charges

\* Susceptibilities of conserved charges

$$\chi_{lmn}^{BSQ} = \frac{\partial^{l+m+n} p / T^4}{\partial(\mu_B/T)^l \partial(\mu_S/T)^m \partial(\mu_Q/T)^n}$$

\* Diagonal second-order susceptibilities measure the response of the **charge density** to an infinitesimal change in the **chemical potential**

$$\chi_2^X = \frac{\partial^2 p / T^4}{\partial(\mu_X/T)^2} = \frac{\partial}{\partial(\mu_X/T)} \left( n_X / T^3 \right)$$

➔ A **rapid increase** of these observables in a certain temperature range signals a **phase transition**

\* **Non-diagonal** susceptibilities measure the **correlation** between different charges

$$\chi_{11}^{XY} = \frac{\partial^2 p / T^4}{\partial(\mu_X/T) \partial(\mu_Y/T)} = \frac{\partial}{\partial(\mu_Y/T)} \left( n_X / T^3 \right)$$

➔ Information about the **strength of the interaction**



# Linking lattice QCD and experiment

\* **Susceptibilities** of conserved charges are the **cumulants** of their event-by event distribution

$$\text{mean : } M = \chi_1$$

$$\text{variance : } \sigma^2 = \chi_2$$

$$\text{skewness : } S = \chi_3/\chi_2^{3/2}$$

$$\text{kurtosis : } \kappa = \chi_4/\chi_2^2$$

$$S\sigma = \chi_3/\chi_2$$

$$\kappa\sigma^2 = \chi_4/\chi_2$$

$$M/\sigma^2 = \chi_1/\chi_2$$

$$S\sigma^3/M = \chi_3/\chi_1$$

\* Lattice QCD results are functions of **temperature** and **chemical potential**

➔ By comparing lattice results and experimental measurement we can **extract the freeze-out parameters from first principles**



# Baryometer and thermometer

\* Let us look at the Taylor expansion of  $R_{31}^B$

$$R_{31}^B(T, \mu_B) = \frac{\chi_3^B(T, \mu_B)}{\chi_1^B(T, \mu_B)} = \frac{\chi_4^B(T, 0) + \chi_{31}^{BQ}(T, 0)q_1(T) + \chi_{31}^{BS}(T, 0)s_1(T)}{\chi_2^B(T, 0) + \chi_{11}^{BQ}(T, 0)q_1(T) + \chi_{11}^{BS}(T, 0)s_1(T)} + \mathcal{O}(\mu_B^2)$$

\* To order  $\mu_B^2$  it is independent of  $\mu_B$ : it can be used as a **thermometer**

\* Let us look at the Taylor expansion of  $R_{12}^B$

$$R_{12}^B(T, \mu_B) = \frac{\chi_1^B(T, \mu_B)}{\chi_2^B(T, \mu_B)} = \frac{\chi_2^B(T, 0) + \chi_{11}^{BQ}(T, 0)q_1(T) + \chi_{11}^{BS}(T, 0)s_1(T)}{\chi_2^B(T, 0)} \frac{\mu_B}{T} + \mathcal{O}(\mu_B^3)$$

\* Once we extract  $T$  from  $R_{31}^B$ , we can use  $R_{12}^B$  to extract  $\mu_B$



# Caveats

- \* Effects due to volume variation because of finite centrality bin width
- \* Finite reconstruction efficiency
- \* Spallation protons
- \* Canonical vs Grand Canonical ensemble
- \* Proton multiplicity distributions vs baryon number fluctuations
- \* Final-state interactions in the hadronic phase



# Caveats

- \* Effects due to volume variation because of finite centrality bin width

  - Experimentally corrected by centrality-bin-width correction method

- \* Finite reconstruction efficiency

  - Experimentally corrected based on binomial distribution

- \* Spallation protons

  - Experimentally removed with proper cuts in  $p_T$

- \* Canonical vs Grand Canonical ensemble

  - Experimental cuts in the kinematics and acceptance

- \* Proton multiplicity distributions vs baryon number fluctuations

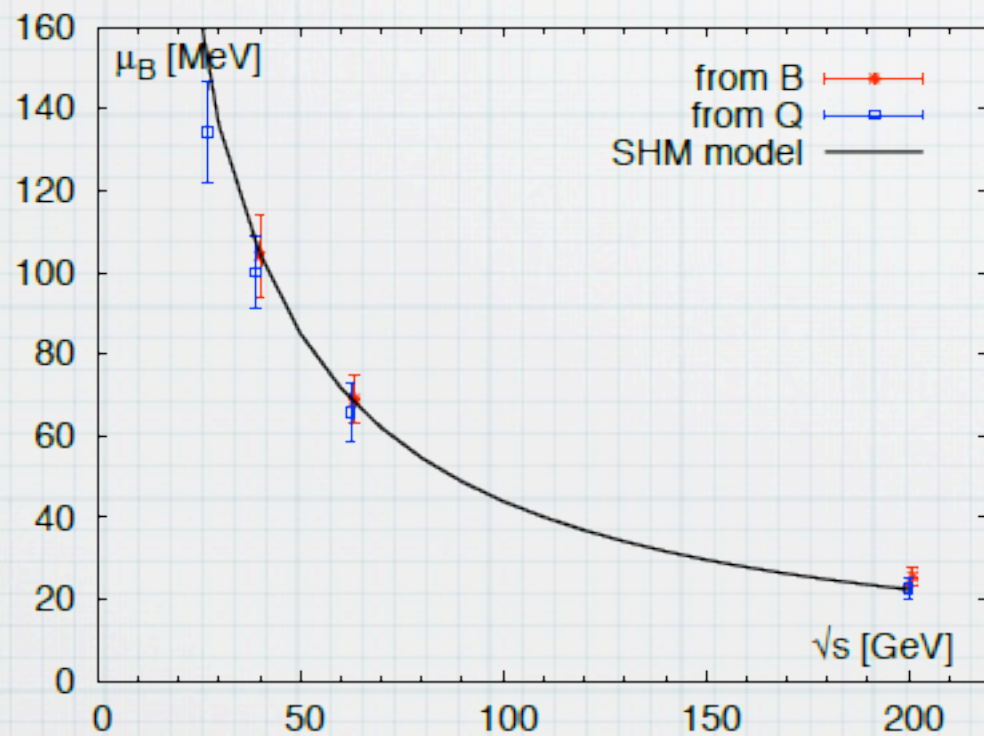
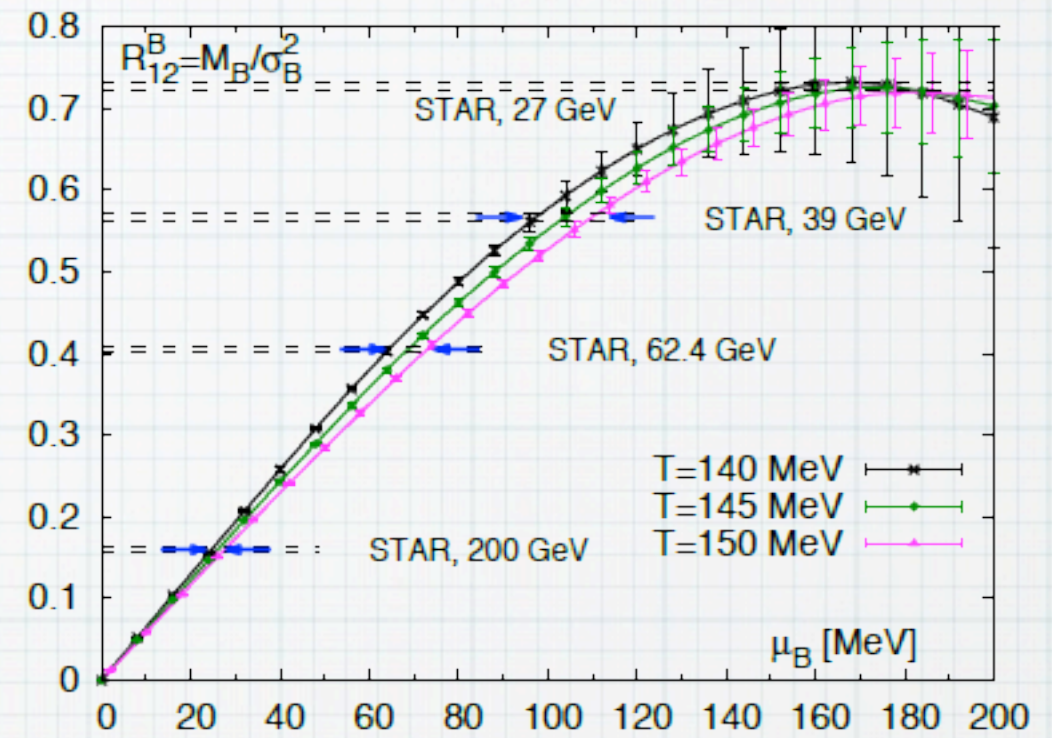
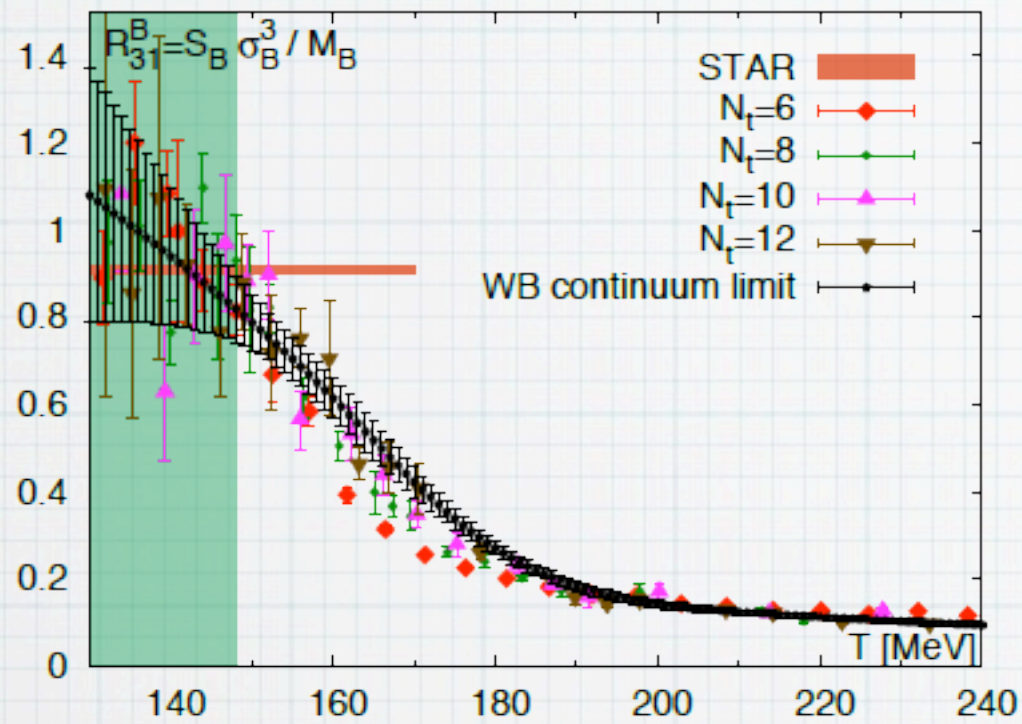
  - Numerically very similar once protons are properly treated

- \* Final-state interactions in the hadronic phase

  - Consistency between different charges = fundamental test



# Results

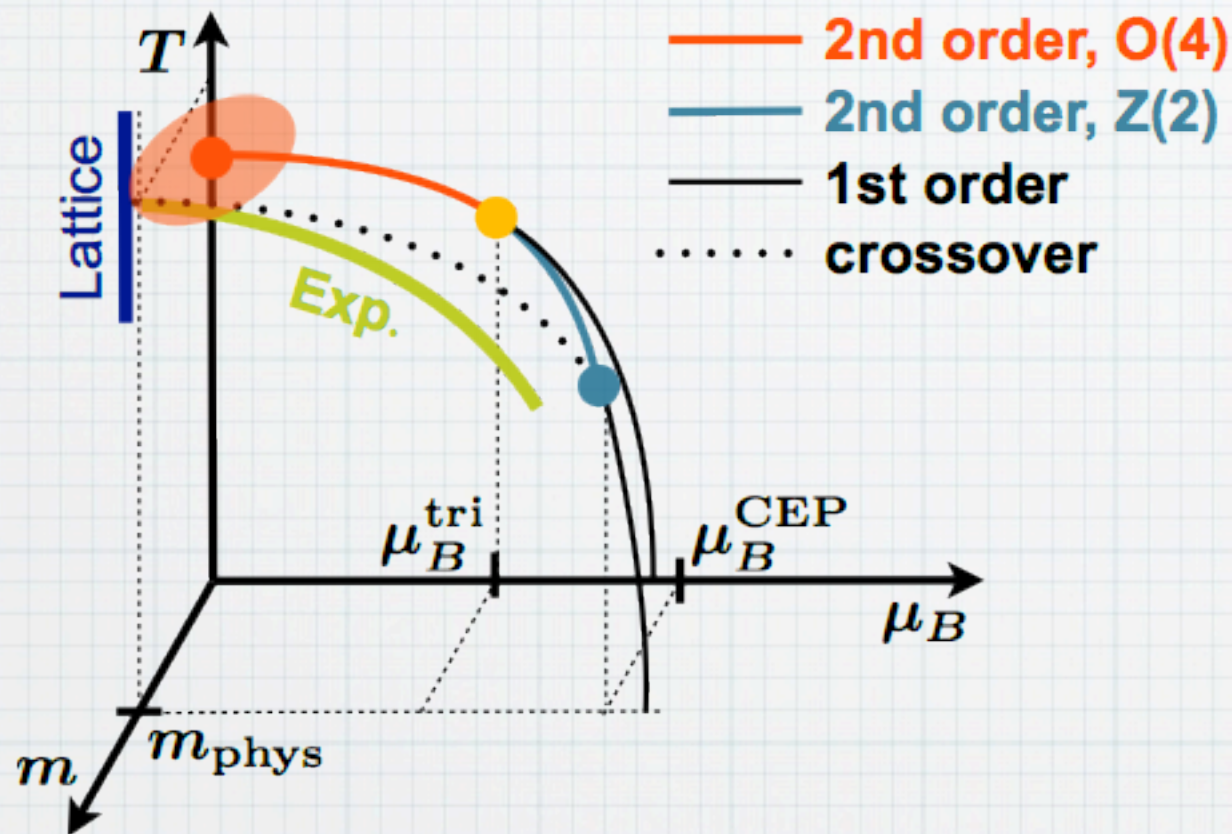


Consistency between  
different charges and  
with SHM fits



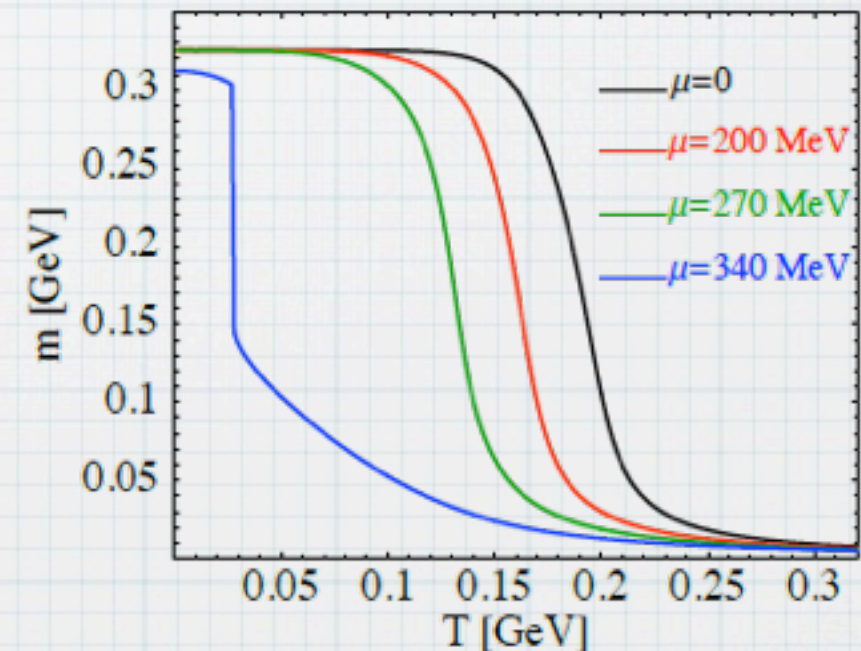
# Our world is not ideal:

neither chiral symmetry ( $m_q=0$ ) nor confinement ( $m_q=\infty$ ) is well defined.



Existence of QCD critical point predicted by models

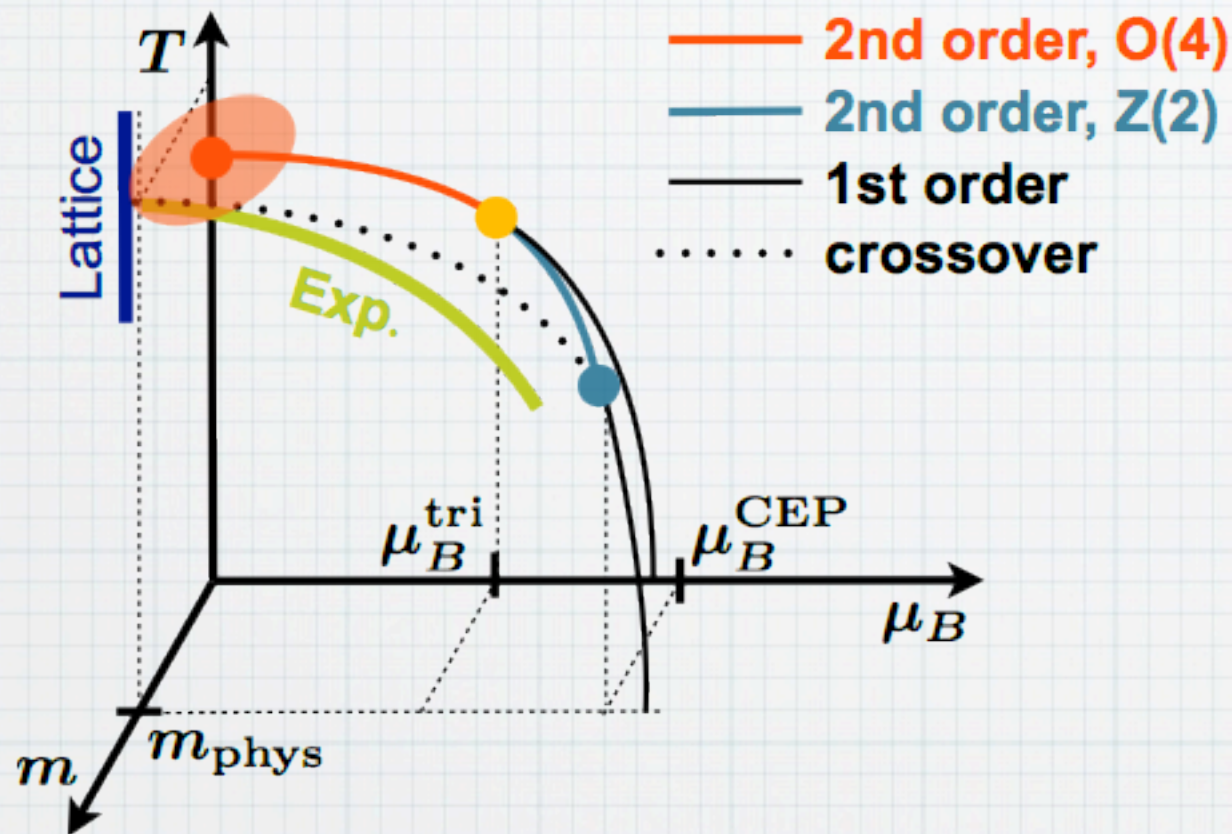
$Z(2)$  universality class





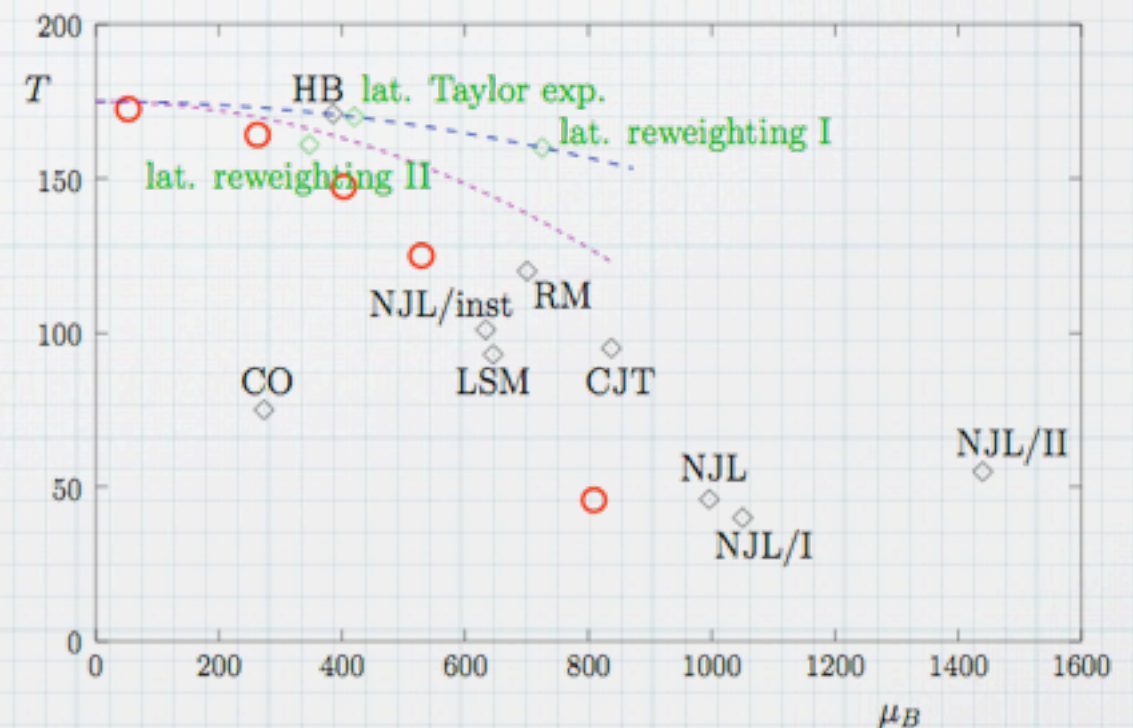
# Our world is not ideal:

neither chiral symmetry ( $m_q=0$ ) nor confinement ( $m_q=\infty$ ) is well defined.



Existence of QCD critical point predicted by models

Z(2) universality class

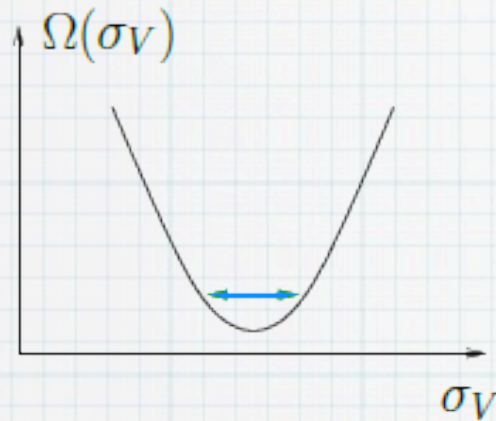




# Fluctuations at the critical point

1

$\mu < \mu_{\text{CP}}$



Consider the order parameter for the chiral phase transition  $\sigma \sim \bar{\psi}\psi$

It has a probability distribution of the form:

2

$\mu = \mu_{\text{CP}}$



$$P[\sigma] \sim \exp\{-\Omega[\sigma]/T\},$$

$$\Omega = \int d^3x \left[ \frac{1}{2}(\nabla\sigma)^2 + \frac{m_\sigma^2}{2}\sigma^2 + \frac{\lambda_3}{3}\sigma^3 + \frac{\lambda_4}{4}\sigma^4 + \dots \right].$$

3

$\mu > \mu_{\text{CP}}$



where:  $m_\sigma \equiv \xi^{-1}$

and, near the critical point:

$$\lambda_3 = \tilde{\lambda}_3 T (T \xi)^{-3/2}, \quad \text{and} \quad \lambda_4 = \tilde{\lambda}_4 (T \xi)^{-1}$$

$$\langle \sigma_V^3 \rangle = 2VT^{3/2} \tilde{\lambda}_3 \xi^{4.5}$$

$$\langle \sigma_V^4 \rangle = 6VT^2 [2(\tilde{\lambda}_3)^2 - \tilde{\lambda}_4] \xi^7$$

correlation length  $\xi$  is **limited** due to critical slowing down, together with the finite time the system has to develop the correlations:  $\xi < 2-3 \text{ fm}$



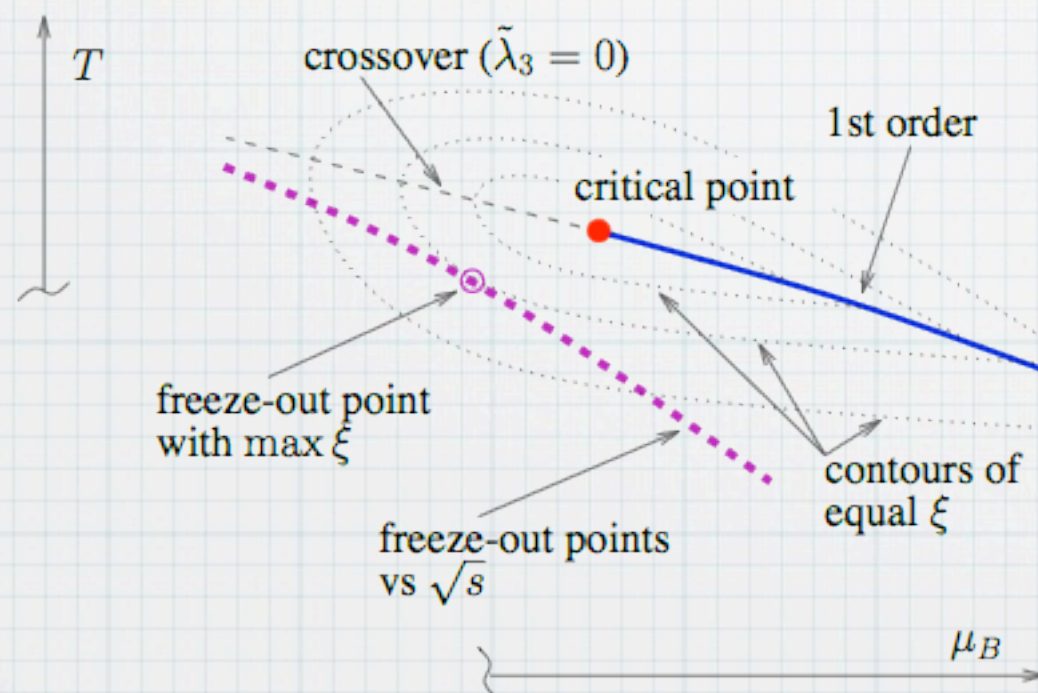
# Experimental fluctuations

We consider the fluctuation of an observable (e.g. protons)

$$\delta N = \sum_{\mathbf{p}} \delta n_{\mathbf{p}}$$

At the critical point, it receives both a regular and a singular contribution. The latter comes from the coupling to the  $\sigma$  field:

$$\delta n_{\mathbf{p}} = \underbrace{\delta n_{\mathbf{p}}^0}_{\text{statistical (Poisson)}} + \underbrace{\frac{\partial \bar{n}_{\mathbf{p}}}{\partial m} g \delta \sigma}_{\text{critical}}$$



Higher order moments have **stronger dependence on  $\xi$** : they are more sensitive signatures for the critical point



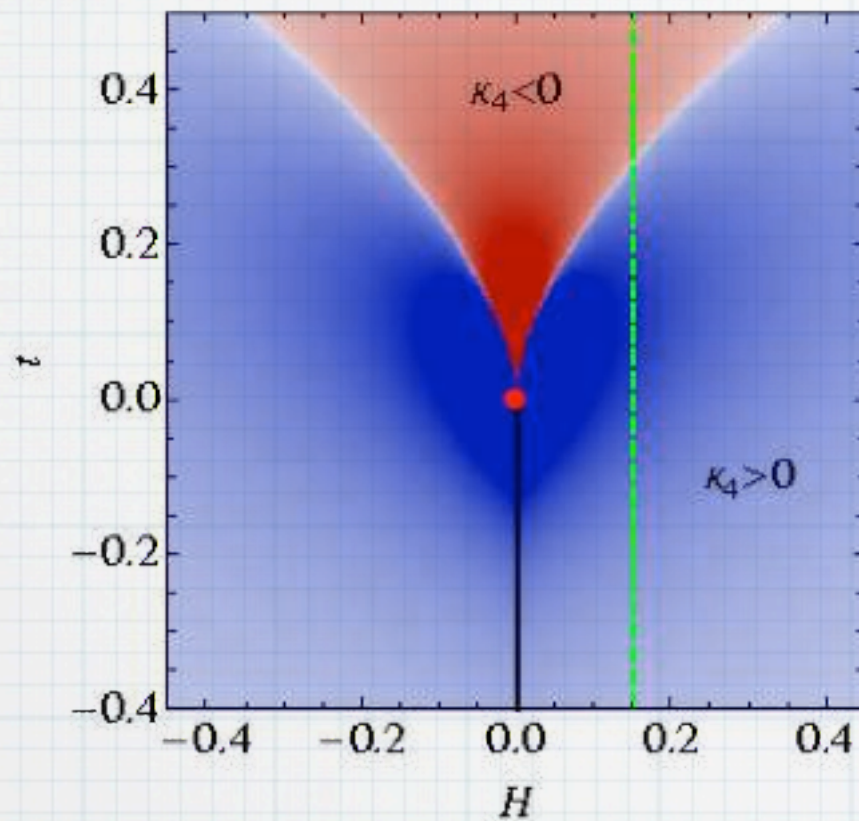
# Sign of kurtosis

The 4th order cumulant becomes **negative** when the critical point is **approached from the crossover side**: from Ising model:

$$M = R^{\beta}\theta, \quad t = R(1-\theta^2), \quad H = R^{\beta\delta}h(\theta)$$

$$K_4 = \langle M^4 \rangle \quad (t, H) \rightarrow (\mu - \mu_{CP}, T - T_{CP})$$

Consequently, the experimental 4th order fluctuation will be **smaller than its Poisson value** (precise value depends on  $\xi$ , on how close the freeze-out occurs to the critical point...)



(a)

