Determination of Critical Exponents in Finite Systems

Walter F.J. Müller
for the
ALADIN Collaboration

Critical Phenomena

Critical Phenomena in a nutshell: $t = \frac{T - T_c}{T_c}$

Property		Fluid	Magnet	Power law
Orderparameter		$\rho_l - \rho_g$	M	Bt^{β}
Susceptibility	χ	$\frac{\partial \rho}{\partial \mu}$	$\frac{\partial M}{\partial H}$	$\Gamma^{\pm} t^{-\gamma}$
Correlation length	ξ			$\xi_0^{\pm} t^{-\nu}$

Exponent relations:

$$\gamma' = \gamma \qquad \nu' = \nu \qquad \ldots$$

$$2 - \alpha = d\nu = 2\beta + \gamma = \beta(1 + \delta) = (\tau - 1)/\sigma$$

$\Longrightarrow$ Only two independent exponents

$\Longrightarrow$ Universality classes

Universal amplitude ratios:

$$\Gamma/\Gamma' = \text{universal} \qquad (\approx 5.0)$$

$$\xi_0^3 \left(\frac{B^2 P_c}{\Gamma k T_c} \right) = \text{universal} \qquad (\approx 0.69)$$

Universal Equation of State:

Only four free parameters

Constituents and Clusters

In the previous talk an attempt was shown to determine

- order parameter $\Delta\rho = \rho_l - \rho_g$
- compressibility $\kappa_T = -\frac{1}{V}\frac{\partial V}{\partial p}$

of a system as a function of a control parameter and to deduce critical exponents from this dependence.

Problem:	Only size and momenta of clusters are known
Needed:	Connection $\Delta\rho, \kappa_T \Longleftrightarrow$ cluster distribution
Solution:	Fisher droplet model and Percolation

1. Step: Fisher's droplet model

$$-\frac{\phi}{kT} = \frac{pV}{kT} = \ln \mathcal{Z} = \sum Y_{(A)}$$

$$Y_{(A)} = q_0 A^{-\tau} \exp\left(-\tfrac{1}{T}\left(sA^{\sigma} - \mu A\right)\right)$$

$$\kappa_T = \frac{T}{V\rho^2}\frac{\partial^2}{\partial\mu^2}\ln \mathcal{Z} = \frac{1}{TV\rho^2}\sum A^2 Y_{(A)}$$

2. Step: Percolation

$\kappa_T \propto M_2$ and $\Delta\rho \propto P_\infty \Longrightarrow$ use percolation theory

Connection $\kappa_T \Longleftrightarrow M_2$

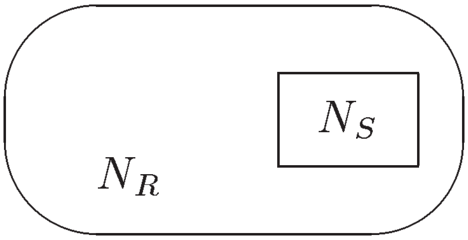
In the Grand canonical ensemble, the compressibility κ_T is related to the fluctuation of the particle number σ_N^2 by

$$\sigma_N^2 = kT \frac{\partial N}{\partial \mu}\bigg|_{T,V} = kT \frac{N^2}{V} \kappa_T$$

with $\kappa_T = -\frac{1}{V}\frac{\partial V}{\partial p}\Big|_{T,N}$.

Goal: Express σ_N^2 in terms of clusters.

Make a System plus Reservoir Ansatz:



N_S: System
N_R: Reservoir
$N = N_R + N_S$

Define $q_i = \begin{cases} 1 & \text{if particle } i \text{ is in } S \\ 0 & \text{if particle } i \text{ is in } R \end{cases}$

With $\overline{q} = \frac{\langle N_S \rangle}{N}$

$$\begin{aligned} \sigma_{N_S}^2 &= \left\langle N_S^2 \right\rangle - \left\langle N_S \right\rangle^2 \\ &= \left\langle \sum_{ij} (q_i - \overline{q})(q_j - \overline{q}) \right\rangle \end{aligned}$$

Now group constituents into clusters.

Assumption 1: $\boxed{\text{A cluster is either in } S \text{ or in } R}$

This allows to split the sum into two parts:

$$\sigma_{N_S}^2 = \left\langle \sum_{\substack{ij\\ \text{same}}} (q_i - \overline{q})(q_j - \overline{q}) \right\rangle + \underbrace{\left\langle \sum_{\substack{ij\\ \text{diff}}} (q_i - \overline{q})(q_j - \overline{q}) \right\rangle}_{\substack{\parallel\\ 0}}$$

Assumption 2: $\boxed{\text{Constituents in different clusters are uncorrelated}}$

Rewrite as sum over clusters: $\displaystyle\sum_{\substack{ij\\ \text{same}}} \rightarrow \sum_{c_i} |c_i|^2$

$$\sigma_{N_S}^2 = (1 - \overline{q})^2 \left\langle \sum_{\substack{c_i\\ \text{S}}} |c_i|^2 \right\rangle + \underbrace{\overline{q}^2 \left\langle \sum_{\substack{c_i\\ \text{R}}} |c_i|^2 \right\rangle}_{\substack{\downarrow\\ 0}}$$

Assumption 3: $\boxed{\text{The largest cluster in } R \text{ grows slower than } N_R \text{ for } N_R \rightarrow \infty \text{ , } \overline{q} \rightarrow 0}$

Finally, with n_s concentration of clusters of size s:

$$\kappa_T = \frac{V}{kT} \frac{\sigma^2_{N_S}}{\langle N_S \rangle^2} = \frac{1}{kT\rho} \sum_s n_s s^2$$

The essential step was assumption 2#:
'Constituents in different clusters are uncorrelated'
which can be paraphrased as
'Clusters do not interact'

For a similar argument see:
Z. Alexandrowicz, Physica **A 160**(1989)310

Ising and Lattice Gas Models

One of the simplest models with a phase transition is the spin 1/2 Ising model with next neighbor interactions:

$$\mathcal{H} = -J \sum_{<i,j>} \sigma_i \sigma_j - H \sum_i \sigma_i$$

Is a model for a magnet or a lattice model of a gas:

	σ_i		E_{int}	
Spins:	$+1$	up	$-2J$	if neighbors aligned
	-1	down	0	otherwise
Sites:	$+1$	occupied	$-2J$	if adjacent sites occupied
	-1	empty	0	otherwise

Equivalences:

$$N \iff V$$
$$M \iff \rho$$
$$H \iff \mu$$

Ensembles:

	Magnet	Lattice Gas
T,H	canonical	grandcanonical
T,M		canonical
E,H	microcanonical	
E,M		microcanonical

$\langle|M|\rangle$ and χ with clusters

Orderparameter $\langle|M|\rangle$ and suszeptibility χ are defined in terms of constituents as:

$$\begin{aligned}
\langle|M|\rangle &= \left\langle\left|\tfrac{1}{N}\textstyle\sum_i \sigma_i\right|\right\rangle \\
\chi &= \tfrac{N}{kT}\left\langle M^2\right\rangle = \tfrac{N}{kT}\left(\tfrac{1}{N^2}\left\langle\textstyle\sum_{ij}\sigma_i\sigma_j\right\rangle\right) \\
\chi' &= \tfrac{N}{kT}\left(\left\langle M^2\right\rangle - \langle|M|\rangle^2\right)
\end{aligned}$$

To express them in terms of clusters, assume the clusters have the properties 1 and 2 of the previous transparency:

Clusters contain only like spins

Clusters are uncorrelated

	n_m	clusters per site with magnetization m
With	m_∞	size of largest cluster
	P_∞	$= \frac{\vert m_\infty\vert}{N}$ fraction of sites in largest cluster

Split n_m in two parts, one with m_∞ and one without

$$n_m = n'_m + \tfrac{1}{N}\delta_{m,m_\infty}$$

Orderparameter:

$$\begin{aligned}
\langle |M| \rangle &= \left\langle \left| \frac{1}{N} \sum_i \sigma_i \right| \right\rangle \\
&= \left\langle \left| \sum_m m\, n_m \right| \right\rangle \\
&= \left\langle \left| \frac{m_\infty}{N} + \sum_m m\, n'_m \right| \right\rangle \\
&\geq \langle P_\infty \rangle
\end{aligned}$$

Suszeptibility for $T \geq T_c$:

$$\begin{aligned}
\chi &= \frac{N}{kT} \left(\frac{1}{N^2} \left\langle \sum_{ij} \sigma_i \sigma_j \right\rangle \right) \\
&= \frac{1}{kT\,N} \left\langle \sum_{\substack{ij \\ \text{same}}} \sigma_i \sigma_j \right\rangle + \underbrace{\frac{1}{kT\,N} \left\langle \sum_{\substack{ij \\ \text{diff}}} \sigma_i \sigma_j \right\rangle}_{=0} \\
&= \frac{1}{kT} \left(\sum_m m^2 \; \langle n_m \rangle \right)
\end{aligned}$$

Suszeptibility for $T < T_c$:

$$
\begin{aligned}
\chi' &= \frac{N}{kT}\left(\langle M^2\rangle - \langle |M|\rangle^2\right) \\
&= \frac{1}{kT}\left(\sum_m m^2\ \langle n'_m\rangle + N\left(\langle P_\infty^2\rangle - \langle |M|\rangle^2\right)\right) \\
&\geq \frac{1}{kT}\left(\sum_m m^2\ \langle n'_m\rangle + N\left(\langle P_\infty^2\rangle - \langle P_\infty\rangle^2\right)\right)
\end{aligned}
$$

With

$$
\begin{aligned}
\chi_p &= \sum_m m^2 < n_m > && \text{Percolation suszeptibility} \\
(\Delta P)^2 &= \langle P_\infty^2\rangle - \langle P_\infty\rangle^2 && \text{Fluctuation of largest cluster}
\end{aligned}
$$

one can write the the cluster observables as # :

$$
\boxed{
\begin{array}{llll}
\widetilde{M} & := \langle P_\infty\rangle & \leq & \langle |M|\rangle \\
\widetilde{\chi} & := \frac{1}{kT}\,\chi_p & = & \chi \\
\widetilde{\chi}' & := \frac{1}{kT}\left(\chi'_p + N(\Delta P)^2\right) & \geq & \chi'
\end{array}
}
$$

See for example:

M. D'Onorio De Meo *et al.*, J. Stat. Phys. **60**(1990)585

Jian-Sheng Wang, Physica **A 161**(1989)249

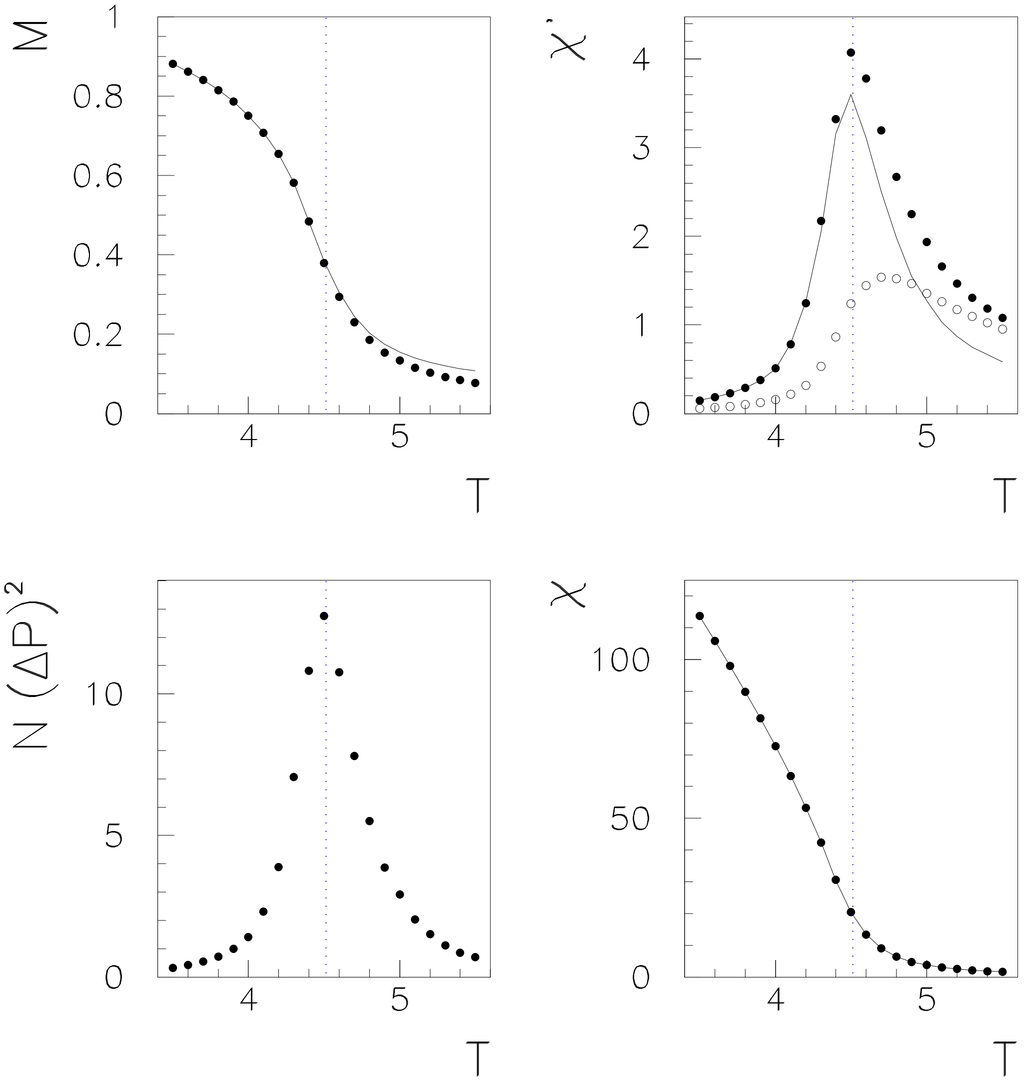
Z. Alexandrowicz, Physica **A 160**(1989)310

Chin-Kun Hu, Phys. Rev. **B 29**(1984)5103

J. Roussenq *et al.*, J. Physique-Lett. **43**(1982)L703

Test Cluster Observables

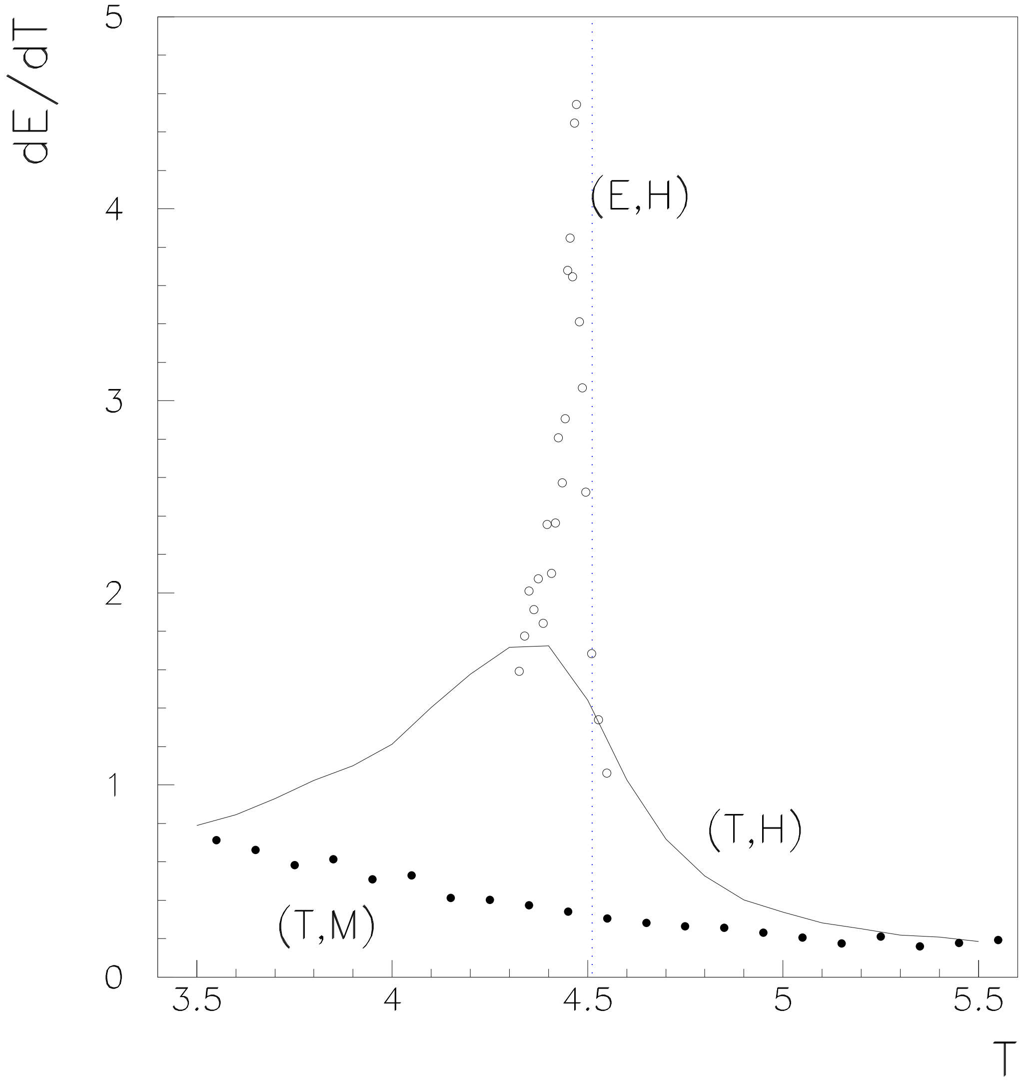
Use the 3d Ising Model with L=8 and periodic bounds.



Note, that the (T,H) ensemble was used.

Differences of Ensembles

Again 3d Ising Model with L=8 and periodic bounds.



Cluster Definitions

'Critical clusters' $\iff$ $M \sim P_\infty$ and $\chi \sim \frac{1}{kT}\sum s^2 n_s$

> Remember:
> 'Critical clusters' have no correlation
> between constituents of different clusters

'Geometrical clusters':

Regions of like spins surrounded by reversed spins.
$\longrightarrow$ an up cluster is surrounded by one down cluster
$\longrightarrow$ correlation $\longrightarrow$ can not be 'critical cluster' $\Downarrow$

'Coniglio-Klein clusters'# **:**

Like spins connected by a bond with $p = 1 - e^{-\frac{2J}{kT}}$

$$\mathcal{Z} = \sum_\sigma e^{-\frac{1}{kT}\mathcal{H}(\sigma)}$$
$$= \sum_c p^{b_c}(1-p)^{N'-b_c}\, 2^{n_c}$$

with $b_c = \#$ of bonds, $n_c = \#$ of clusters

$\longrightarrow$ No correlation $\longrightarrow$ is proper 'critical cluster' $\Uparrow$

A. Coniglio and W. Klein, J. Phys. **A 13**(1980)2775
P.W. Kastelyn and C.M. Fortuin, J. Phys. Soc. Japan **26**(1969)11

Gedankenexperiment:

- Start with a cluster configuration c_1
- Create c_2 by reversing spins in one cluster
- The interaction energy is in general not zero

$$E(c_1) \neq E(c_2)$$

- Both configurations have the same probability

$$p(c_1) = p(c_2)$$

- Reason:

$$\Omega_{(E(c_1))} e^{-\frac{E(c_1)}{kT}} = \Omega_{(E(c_2))} e^{-\frac{E(c_2)}{kT}}$$

The critical clusters are
interacting and uncorrelated !

Question:
Are ‘Critical clusters’ observable entities
or just a mathmatical construction ?

Dependence on T and χ' Prescription

Use an analysis very similar to the Purdue method.
But take into account:

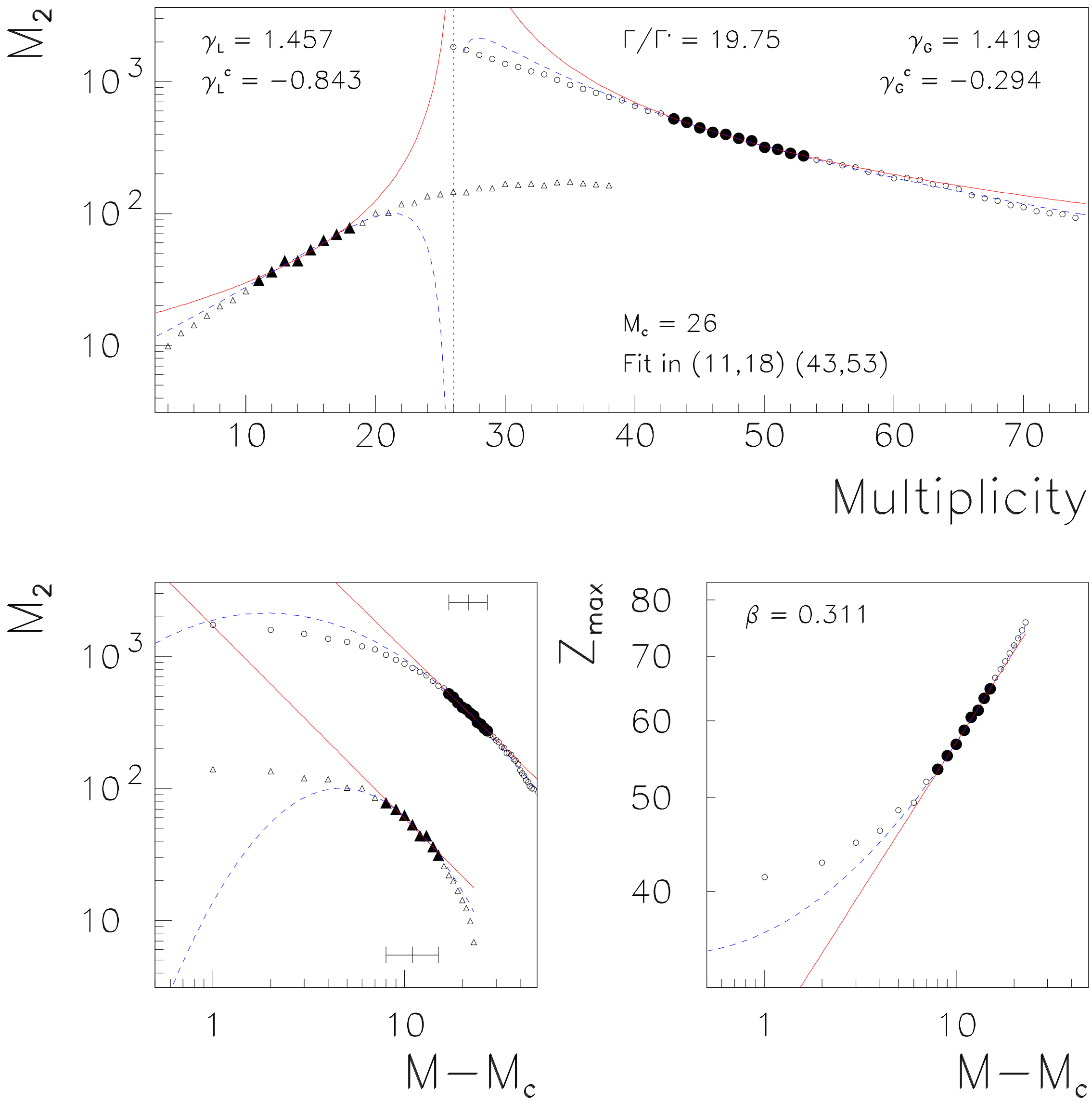
- the $\frac{1}{kT}$ factor
- the fluctuation of the largest fragment: $N(\Delta P)^2$

Use 3 parametrizations for T:

'$T_{\rm const}$'	$T \propto 1$
'$T_{\rm final}$'	$T \propto 1 + 0.01\,(M - 30)$
'$T_{\rm initial}$'	$T \propto 1 + 0.02\,(M - 30)$

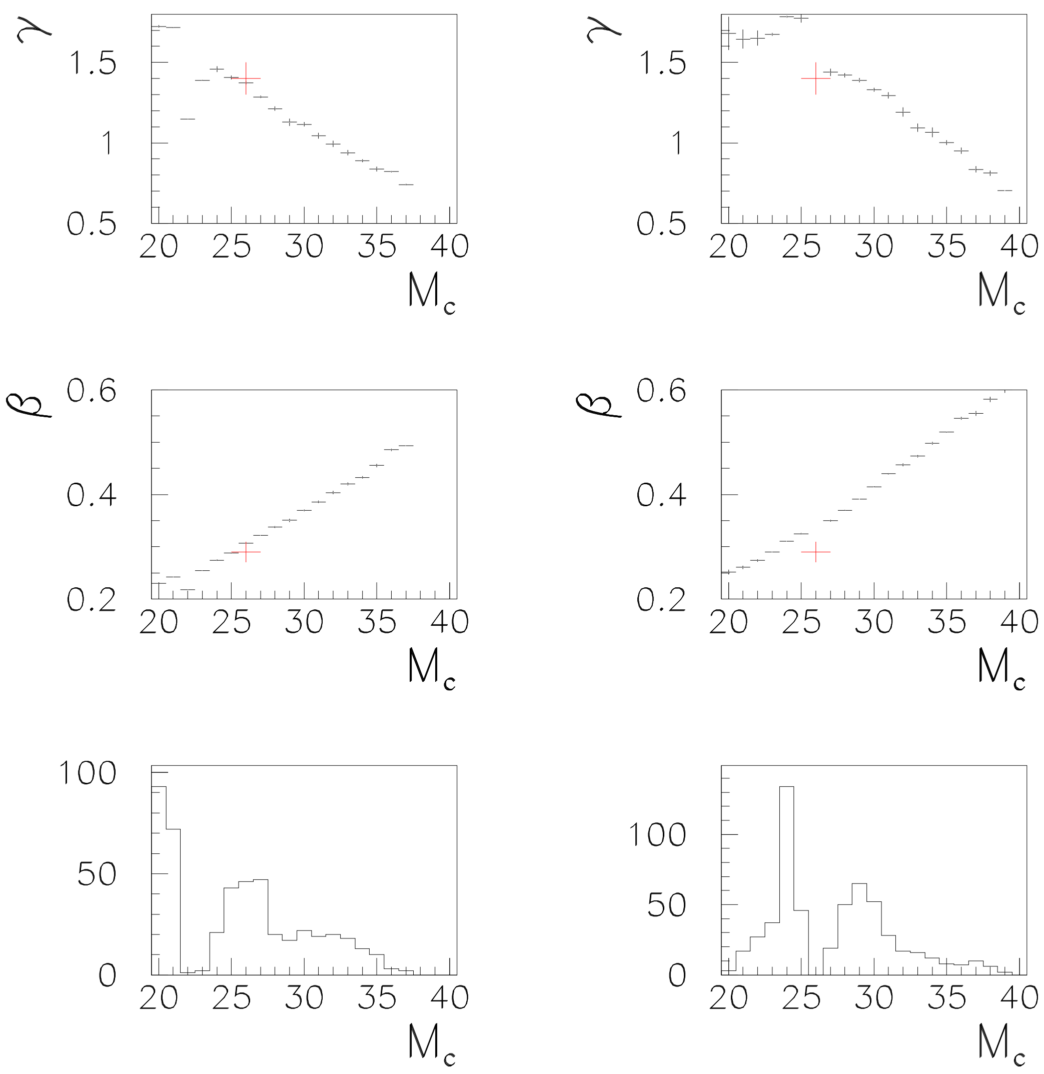
Use ALADIN data: 1 A GeV Au + C

Typical Fit 1



$$\chi' = \chi_p$$
$$T \propto const$$

Vary T Parametrization

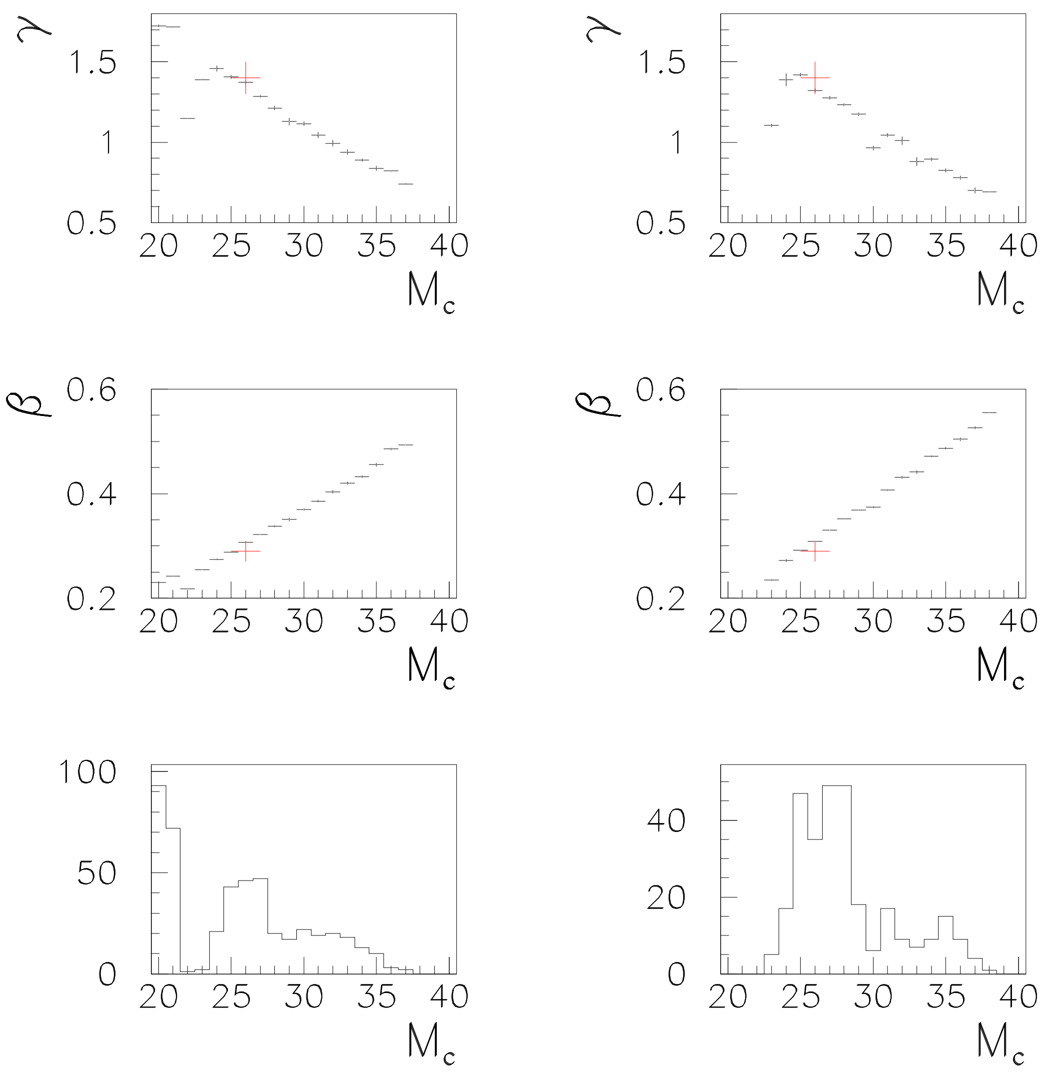


$T \propto const$ $\qquad$ $T \propto 1 + 0.02\,(M - 30)$

Crosses: Gilkes *et al.* results

$$M_c = 26 \pm 1 \qquad \gamma = 1.4 \pm 0.1 \qquad \beta = 0.29 \pm 0.02$$

Vary χ' Prescription

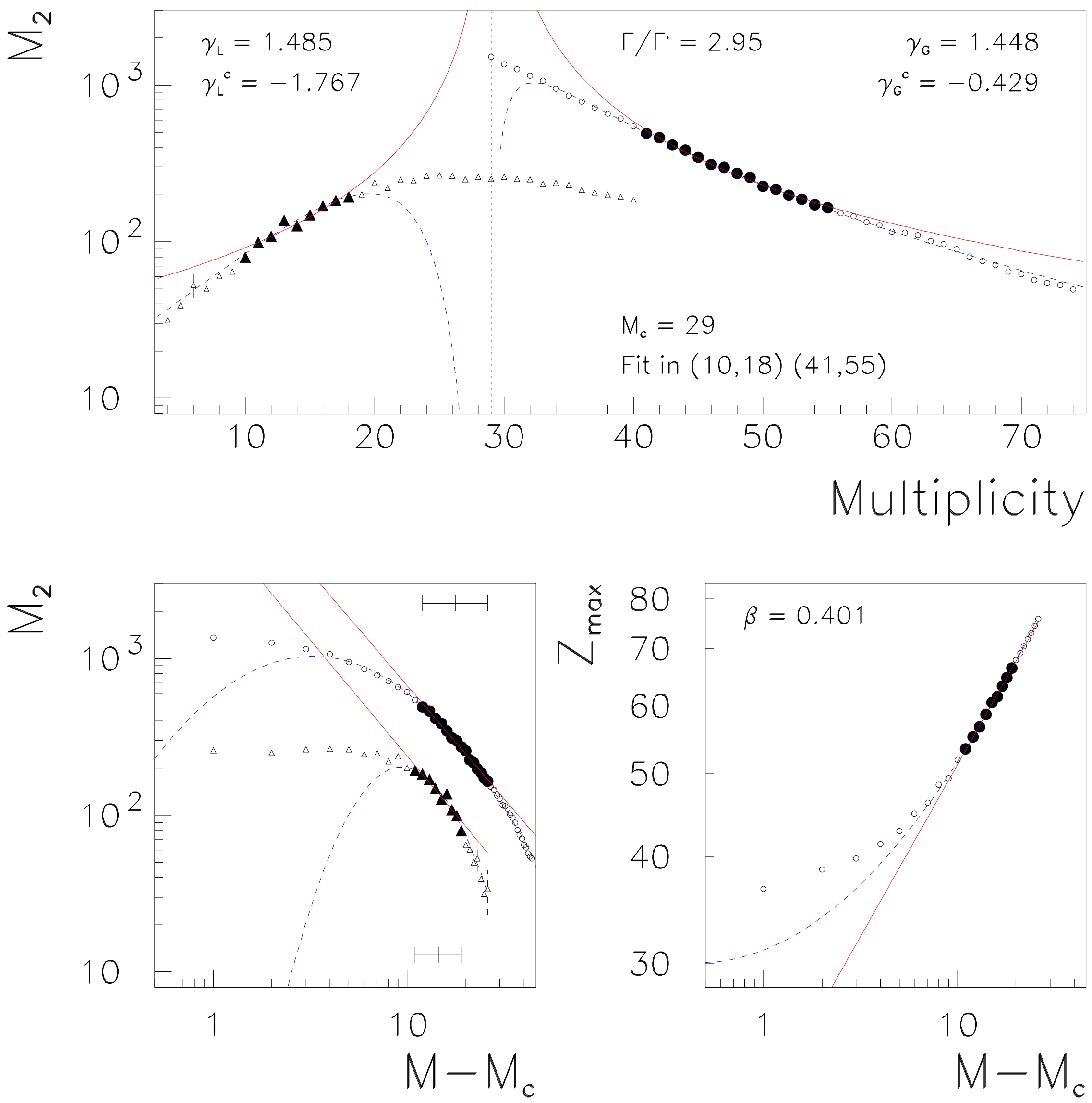


Left panel: $\chi' = \chi_p$

Right panel: $\chi' = \chi_p + N(\Delta P_\infty)^2)$

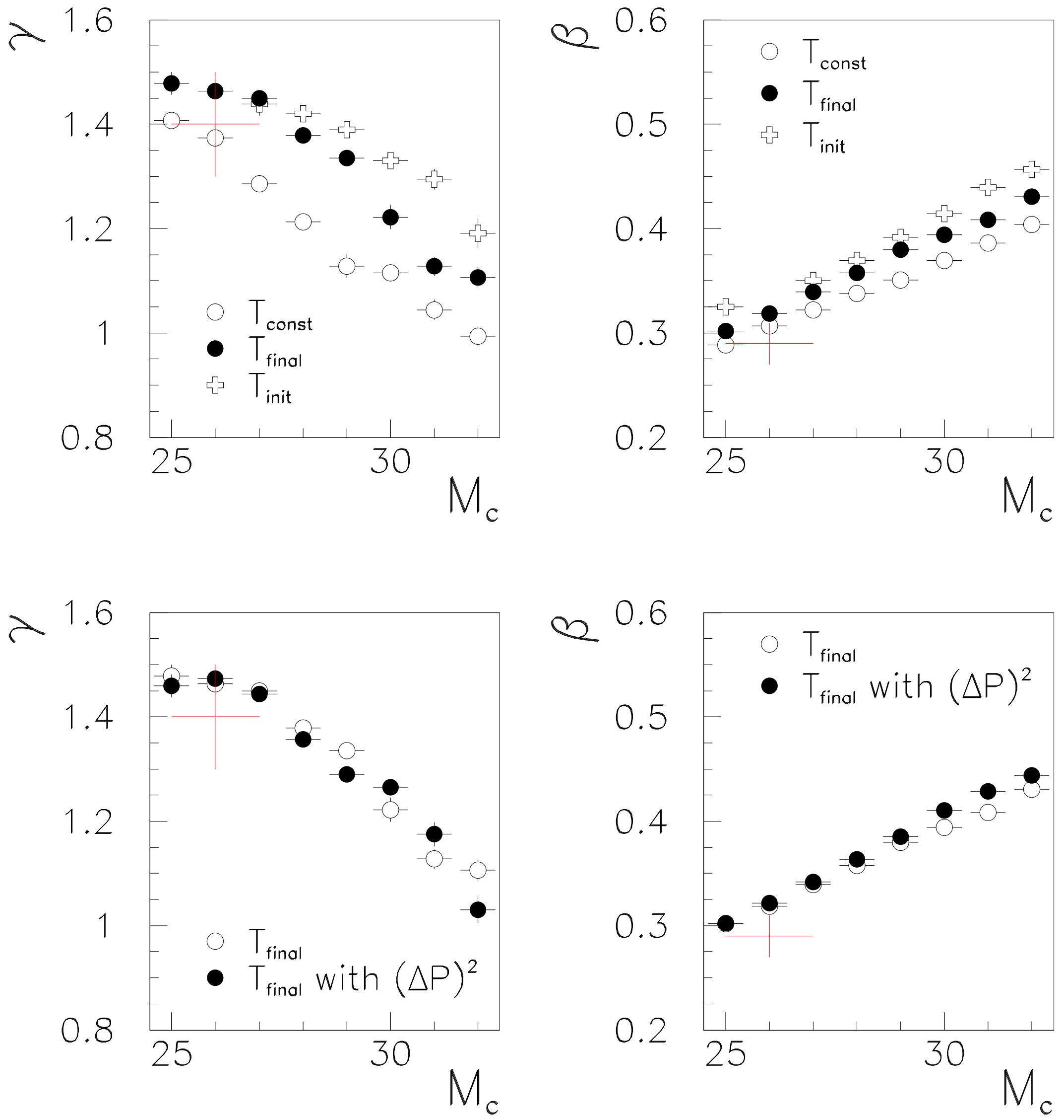
Assumed: $T \propto const$

Typical Fit 2



$$\chi' = \chi_p + N(\Delta P_\infty)^2)$$
$$T \propto 1 + 0.02\,(M - 30)$$

T and χ' Summary



$\Longrightarrow$ γ **and** β **depend on** M_c **choice**

$\Longrightarrow$ M_c **choice depends on** T **parametrization**

$\Longrightarrow$ χ' **prescription affects only** Γ'/Γ

Exponent Extraction

The Purdue method varies five parameters:

- M_c critical multiplicity
- distance of gas and liquid fit interval
- width of gas and liquid fit interval

and uses three contraints or selections:

- M_c choosen e.g. by maximum of $\sigma_{Z_{\max}}$
- $\gamma' = \gamma$
- good reduced χ^2 of combined fit

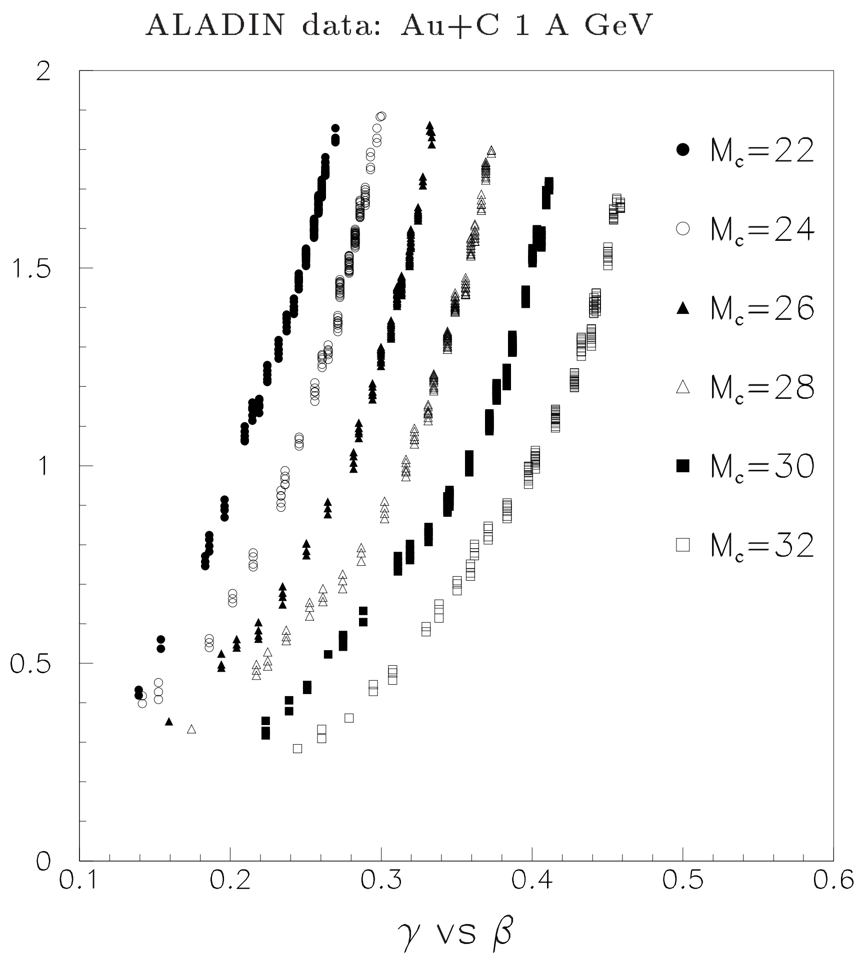
$\Longrightarrow$ Difficult to visualize dependencies

$\Longrightarrow$ Try a simplified, more schematic method

A Schematic Method

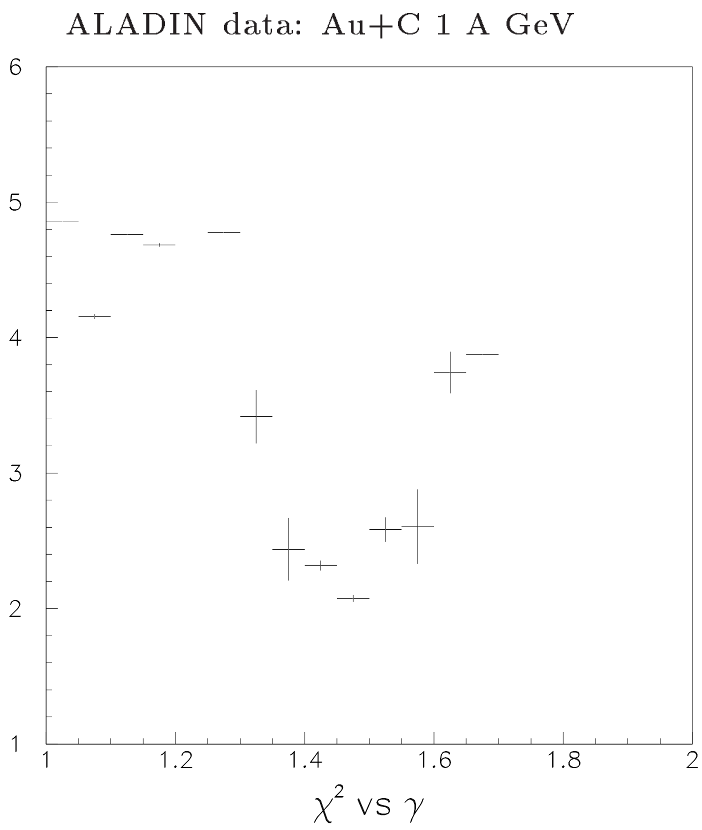
- Fix fit interval width: $\Delta \ln(M - M_c) \approx \ln 2$
- Vary: M_c and distance of gas and liquid fit interval
- Require: $\gamma' = \gamma$

$\Longrightarrow$ For given M_c one gets a γ vs. β relation:



Schematic Method II

Now choose $M_c = 26$, check reduced χ^2 of combined fits:



But: β depends strongly on the choice of M_c

χ^2 minimum is rather shallow

Does χ^2 selection even make sense ?

All other uncertainties ignored so far:

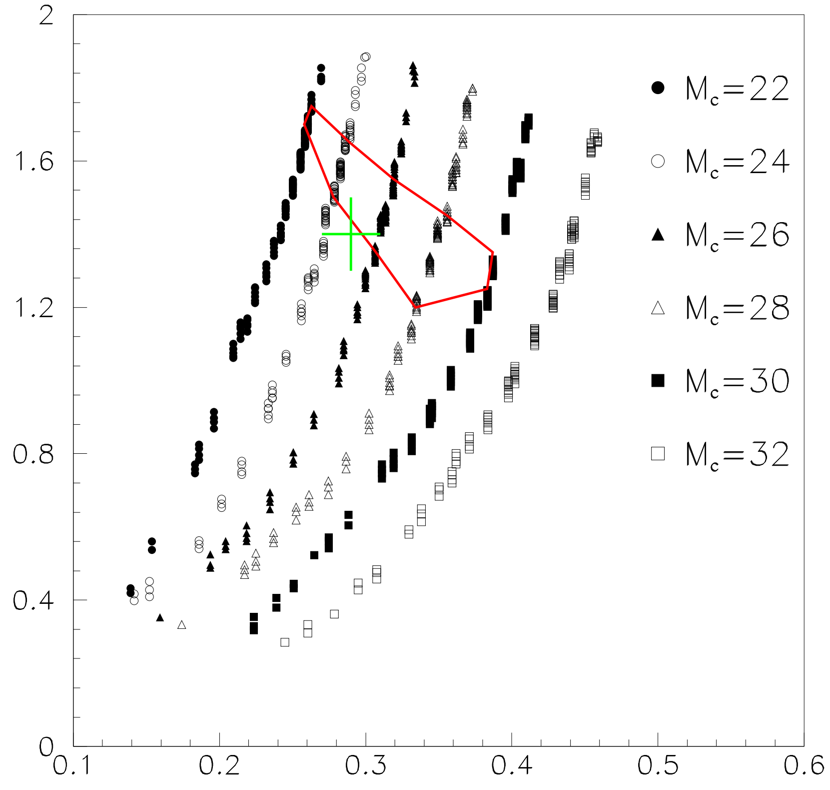
.... varying source size

.... choice of initial parameter space

Schematic Method III

Vary M_c and map out region of χ^2 minimum:

ALADIN data: Au+C 1 A GeV



γ vs β

$\Longrightarrow$ **What are the systematical errors ?**

From Gases to Nuclei

Use the principle of corresponding states: #

> The equation of state, in reduced units, should be universal, except for quantum corrections, which depend on $\lambda = \sqrt{\frac{h^2}{m\epsilon\sigma^2}}$

Typical values for $\lambda \approx$

3	nuclear matter
2.7	^{4}He
3.5	^{3}He

Nuclear matter should be similar to liquid Helium.

The critical amplitudes for the nuclear system, in reduced units, should therefore be similar to the values found for simple liquids:

Typical values are

System	$\xi_0 \rho_c^{1/3}$	Γ
Xe	0.32	0.057
^{4}He	0.45	0.12
^{3}He	0.52	0.15

R. G. Palmer and P. W. Anderson, Phys. Rev. **D 9**(1974)3281

Finite System Size

The correlation length diverges like $\xi = \xi_0 t^{-\nu}$. This should be small compared to the system size $(N/\rho_c)^{1/3}$:

$$\xi_0 \rho_c^{1/3}\, t^{-\nu} < N^{1/3}$$

The scale factor ξ_0 is related to critical amplitudes by

$$\begin{aligned} \xi_0^3 \left(\frac{B^2 P_c}{\Gamma k T_c}\right) &= R \approx 0.69 \\ \xi_0 \rho_c^{1/3} &= R \left(\frac{\Gamma}{r_c B^2}\right)^{\frac{1}{3}} \qquad \text{with } r_c = \tfrac{P_c}{\rho_c k T_c} \end{aligned}$$

Using $\left\{ \begin{array}{rcl} \xi_0 \rho_c^{1/3} & = & 0.5 \\ t & = & 0.3 \\ N & = & 150 \end{array} \right\} \Longrightarrow 1 \approx \xi < N^{1/3} \approx 5.3$

Only 20% of the system is more than one ξ away from the surface.
$\Longrightarrow$ **Surface effects should be important !**

Coulomb Effects

External fields, like gravity or Coulomb, cause a large density gradient when a system is near the critical point.[#]

$$\chi_T = \left.\frac{\partial \rho^\star}{\partial \mu^\star}\right|_T = \Gamma\, t^{-\gamma} \qquad \text{with} \quad \rho^\star = \frac{\rho}{\rho_c} \quad \mu^\star = \frac{\mu \rho_c}{P_c}$$

The relative density change should be small

$$\begin{aligned} \Delta\rho^\star &= \Gamma t^{-\gamma}\, \Delta\mu^\star \ll 1 \\ \Delta\mu &\ll \frac{r_c\, kT_c}{\Gamma\, t^{-\gamma}} \qquad \text{with } r_c = \tfrac{P_c}{\rho_c kT_c} \end{aligned}$$

$$\text{Using} \quad \left\{ \begin{array}{ccc} r_c & = & 0.3 \\ \Gamma & = & 0.12 \\ kT_c & = & 10\ \text{MeV} \\ t & = & 0.3 \end{array} \right\} \Longrightarrow \Delta\mu \ll 5.6\text{MeV}$$

Compare this to the change of the Coulomb potential inside a uniformly charged sphere.

$$\text{Using} \quad \left\{ \begin{array}{ccc} Z & = & 60 \\ A & = & 150 \\ \rho & = & \frac{1}{3}\rho_0 \end{array} \right\} \Longrightarrow \Delta\mu \approx 5\text{MeV}$$

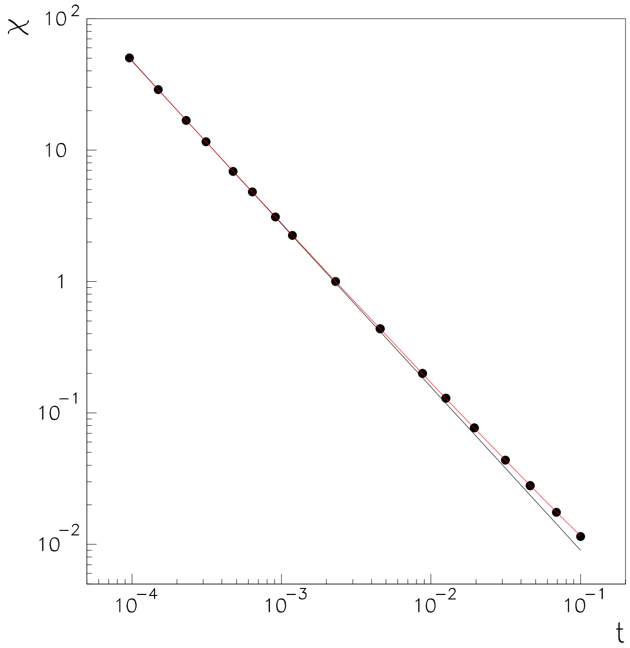
$\Longrightarrow$ **Coulomb effects should be important !**

[#] M.R. Moldover *et al.*, Rev. Mod. Phys. **51**(1979)79

Corrections to Scaling

Power laws hold only **asymtotically** for $t \to 0$.

Example: Suszeptibility of Xenon for $10^{-4} < t < 10^{-1}$:



Data from: H. Güttinger and D.S. Cannell, Phys. Rev. **A24**(1981)3188

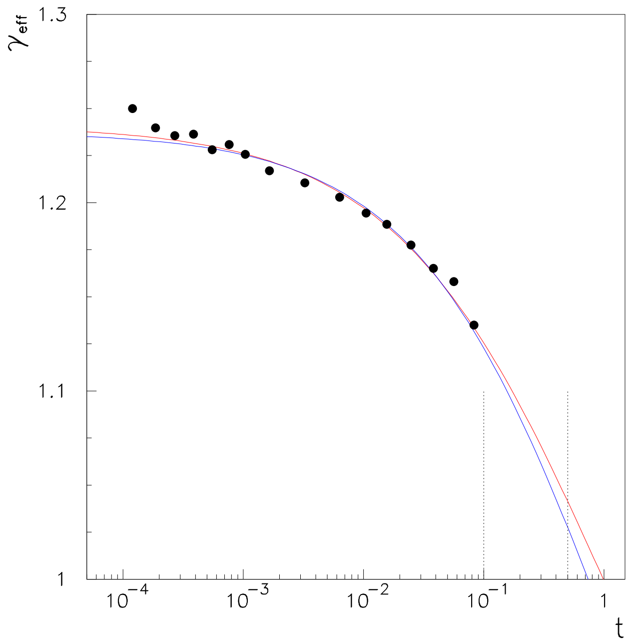
$\Longrightarrow$ use $\chi = \Gamma t^{-\gamma}\left(1 + a_1^\chi t^\Delta + a_2^\chi t^{2\Delta} + \ldots\right)$ with $\Delta \approx 0.49$.

$\Longrightarrow$ or face effective exponents, like $\gamma^{\mathrm{eff}}_{(t)} = -\frac{\partial \ln \chi}{\partial \ln t}$:

$$\begin{aligned} \gamma^{\mathrm{eff}}_{(t)} &\approx \gamma - a_1^\chi \Delta t^\Delta && \Longrightarrow \gamma^{\mathrm{eff}} \text{ smaller} \\ \beta^{\mathrm{eff}}_{(t)} &\approx \beta + a_1^\beta \Delta t^\Delta && \Longrightarrow \beta^{\mathrm{eff}} \text{ larger} \end{aligned}$$

Note, that exponent scaling relations still hold approximately because $\frac{a_1^\gamma}{a_1^\beta} \approx -\frac{\gamma - \gamma_0}{\beta - \beta_0} \approx 1.4$.

Effective Exponents



Data from: H. Güttinger and D.S. Cannell, Phys. Rev. **A24**(1981)3188

Typical correction amplitudes

System	a_1^χ	Ref.
Xe	1.3	H. Güttinger *et al.*, Phys. Rev. **A24**(1981)3188
Ne	1.1	M.W. Pestak *et al.*, Phys. Rev. **B30**(1984)274
N_2	1.1	"
Ising $s = \infty$	0.27	D.M. Saul *et al.*, Phys. Rev. **B11**(1975)2571
Ising $s = \frac{1}{2}$	≈ 0	"

Real gases have $a_1^\chi \approx 1$, some models $a_1^\chi \approx 0$!

$\Longrightarrow$ **Correction terms should be important !**

Scaling Function and τ_{eff}

The proper scaling form of the cluster size distribution on the the coexistence line is

$$n_s = q_0 s^{-\tau} f(ts^\sigma) \qquad \text{with} \quad t = \begin{cases} \frac{T-T_c}{T_c} & \text{thermal} \\ p - p_c & \text{percolation} \end{cases}$$

Characterize the shape of n_s by a **local** powerlaw

$$\tau_{\text{eff}(s,t)} := -\frac{\partial \ln n_{s_{(t)}}}{\partial \ln s}$$

Then τ_{eff} depends only on scaling variable $z = ts^\sigma$

$$\tau_{\text{eff}(s,t)} = \tau - \sigma z \, \frac{\partial}{\partial z} \ln f_{(z)}$$

For a parabolic shape of $\ln f$:

$$\begin{array}{rcll} \ln f_{(0)} & = & 0 & \text{zero} \\ \ln f_{(z_m)} & = & f_m & \text{maximum} \end{array}$$

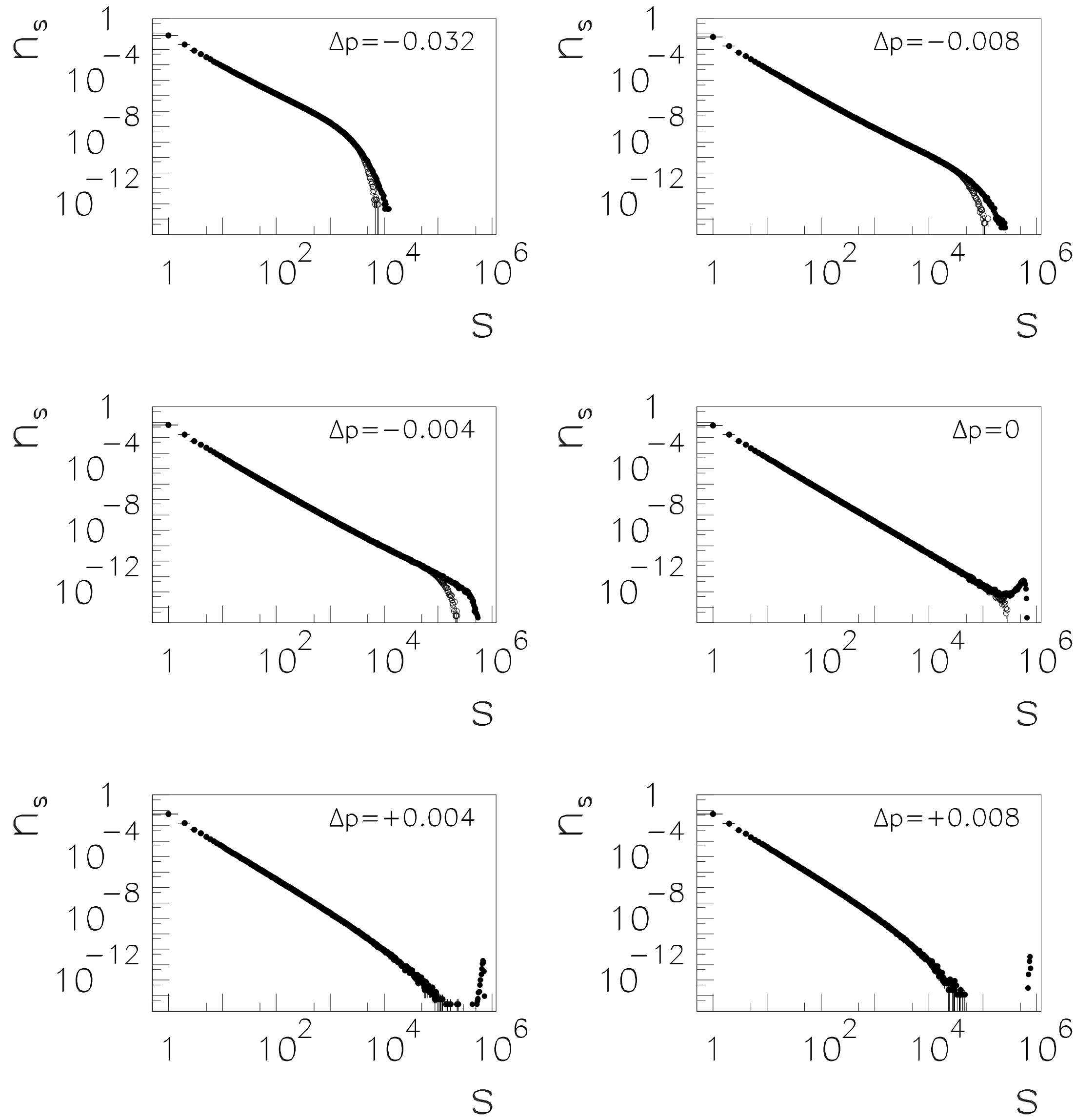
one gets a **minimum of τ_{eff}** with

$$\tau_{\text{eff}}^{\text{min}} = \tau - \frac{\sigma f_m}{2} \qquad \text{at} \qquad z_{\text{min}} = \frac{z_m}{2}$$

$\tau_{\text{eff}}^{\text{min}} < \tau$ and found on the disordered side !

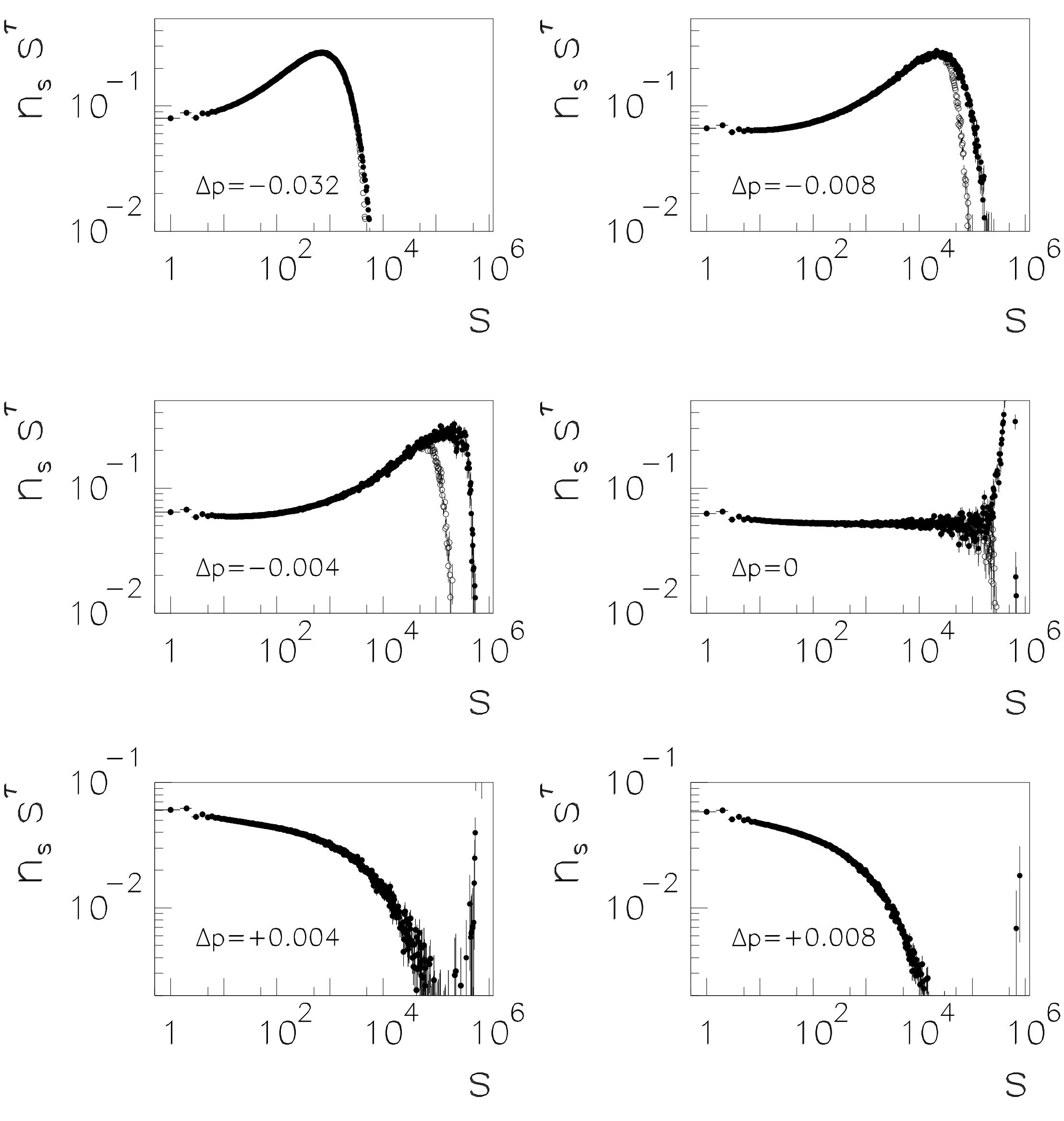
$\tau_{\text{eff}}^{\text{min}}$ relates to the maximum of the scaling function !

Scaling Function and τ_{eff}
Example in 2d Percolation



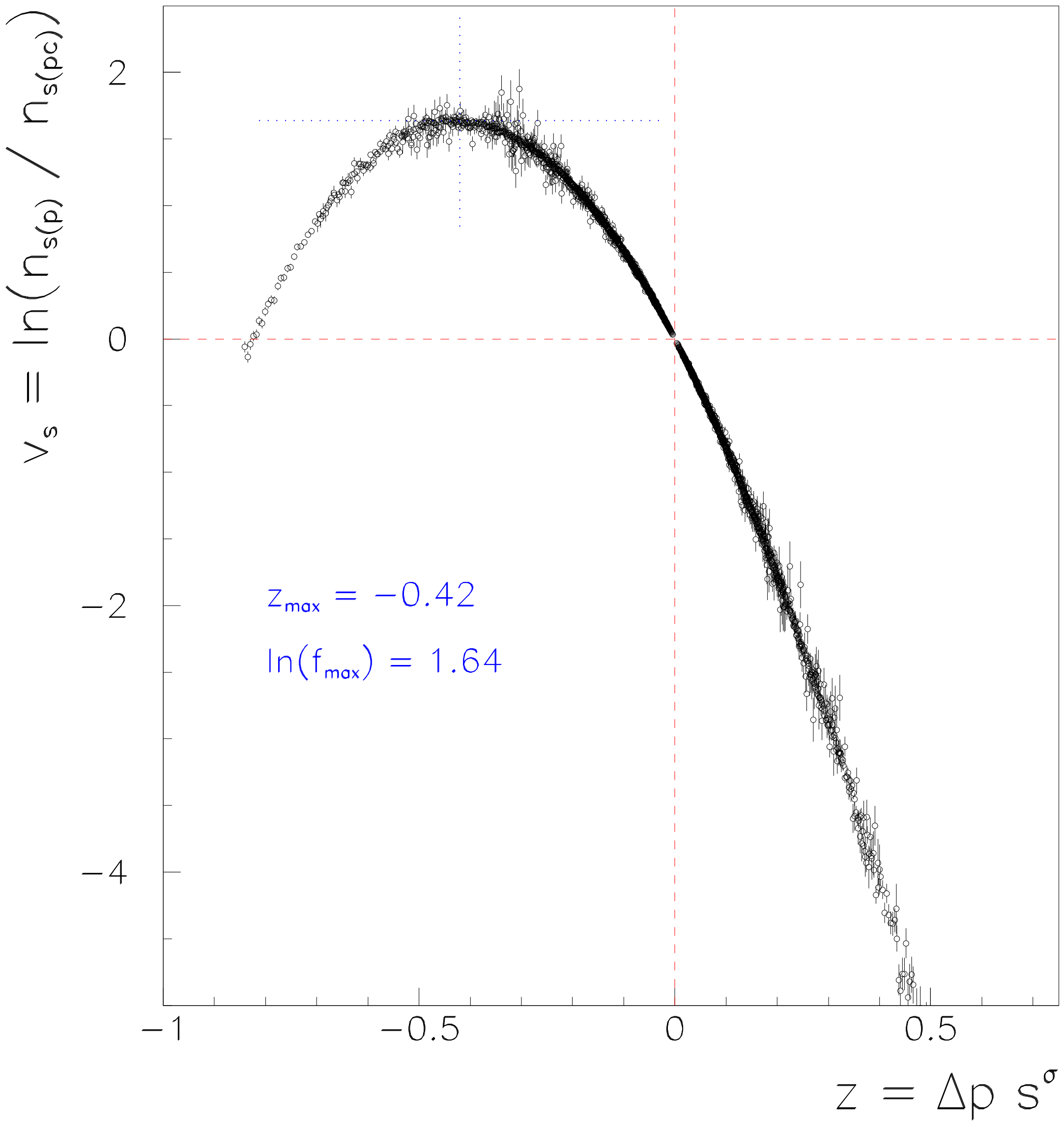
1024*1024 grid; periodic boundary conditions

Deviations from Power law near p_c



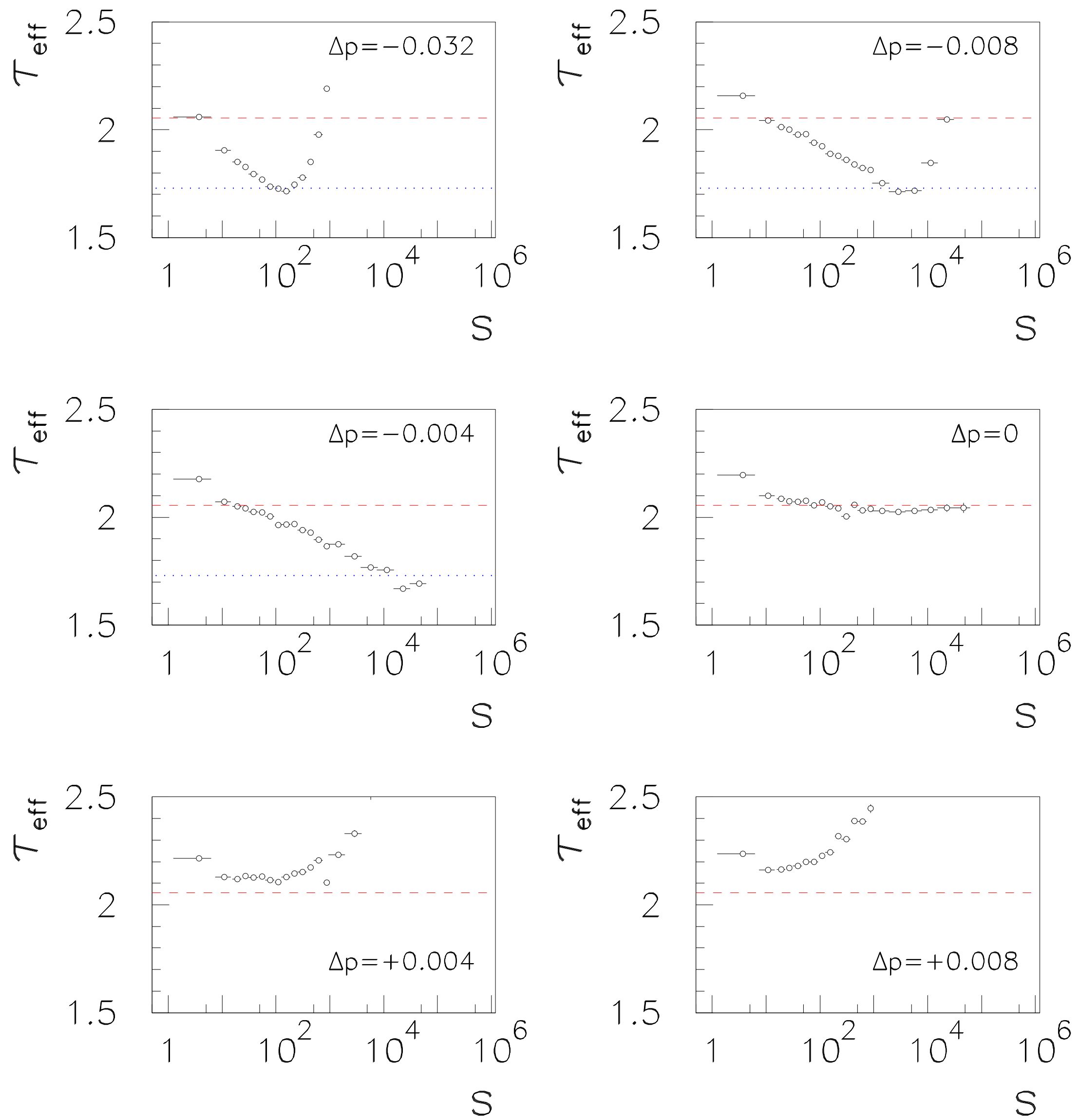
Parameters and exponents for 2d percolation are known exactly: $p_c = \frac{1}{2}$, $\tau = \frac{187}{91}$ and $\sigma = \frac{36}{91}$.

Scaling function for 2d Percolation



Data for $\Delta p = \pm 0.032, \pm 0.016, \pm 0.008$ and ± 0.004

τ_{eff} Fits



One expects $\tau_{\text{eff}}^{\text{min}} \approx 1.73$ and a minimum at $\Delta p s^{\sigma} \approx -0.22$.

Concluding Questions and Remarks

Are critical clusters observable objects ?

Look beyond Percolation !

How well can we determine critical exponents ?

How to interpret critical exponents ?

ALADIN Collaboration

M. Begemann-Blaich, H. Emling, C. Groß, G. J. Kunde,[†]
W. D. Kunze, V. Lindenstruth,[‡] U. Lynen,
W. F. J. Müller, J. Pochodzalla,[§] B. Ocker, Th. Rubehn,[‡]
H. Sann, C. Schwarz, V. Serfling, J. Stroth,
W. Trautmann, A. Wörner, E. Zude

Gesellschaft für Schwerionenforschung, Darmstadt

A. Schüttauf

Institut für Kernphysik, Universität Frankfurt

Th. Blaich

Institut für Kernchemie, Universität Mainz, Mainz

T. Möhlenkamp, W. Seidel

Forschungszentrum Rossendorf, Dresden

R. Bassini, A. Ferrero, I. Iori, A. Moroni

Dipartimento di Fisica, Università di Milano and I.N.F.N., Milano

G. Immé, G. Raciti, G. Verde

Dipartimento di Fisica dell' Università and I.N.F.N., Catania

A. Trzcinski, B. Zwieglinski

Soltan Institute for Nuclear Studies, Warsaw

†Present address: NSCL, MSU, East Lansing
‡Present address: LBNL, Berkeley
§Present address: MPI für Kernphyik, Heidelberg