Connecting grand-canonical cumulants of conserved charges to experiment

Volodymyr Vovchenko (LBNL)

Workshop on event-by-event fluctuations (virtual)

September 15, 2020

• Subensemble acceptance method (SAM)

• Particlization routine for event-by-event fluctuations
  V.V., V. Koch, to appear
Relativistic heavy-ion collisions

Event display of a Pb-Pb collision in ALICE at the LHC

Thousands of particles created in relativistic heavy-ion collisions

Apply concepts of statistical mechanics
Event-by-event fluctuations: Motivations

Grand-canonical ensemble: \( \kappa_n = \frac{1}{\sqrt{T^3}} \chi^n_B(T, \mu) \), \( \chi^n_B(T, \mu) = \frac{\partial^n(p/T^4)}{\partial(\mu_B/T)^n} \)

- **QCD critical point** [M. Stephanov, PRL ‘09]
  \( \kappa_2 \sim \xi^2, \quad \kappa_3 \sim \xi^{4.5}, \quad \kappa_4 \sim \xi^7, \quad \xi \rightarrow \infty \)

  NA61/SHINE, STAR-BES

- **Chiral criticality** at \( \mu_B = 0 \)
  - Higher-order baryon number susceptibilities

    LHC Runs 3 & 4 [1812.06772]

- **Comparisons with first-principle lattice QCD predictions**
  (fluctuations of conserved charges)

  - Direct comparisons of experimental data with grand-canonical fluctuations from different theories is commonplace: lattice QCD (Wuppertal-Budapest; HotQCD), HRG (Houston group; Nahrgang, Bluhm;...), effective QCD approaches (Fischer et al.; Pawlowski et al.),...
Theory vs experiment: Caveats

- proxy observables in experiment (net-proton, net-kaon) vs actual conserved charges in QCD (net-baryon, net-strangeness)
  Asakawa, Kitazawa, PRC ’12; V.V., Jiang, Gorenstein, Stoecker, PRC ’18

- volume fluctuations
  Gorenstein, Gazdzicki, PRC ’11; Skokov, Friman, Redlich, PRC ’13;
  Braun-Munzinger, Rustamov, Stachel, NPA ’17

- non-equilibrium (memory) effects
  Mukherjee, Venugopalan, Yin, PRC ’15

- final-state interactions in the hadronic phase
  Steinheimer, V.V., Aichelin, Bleicher, Stoecker, PLB ’18

- accuracy of the grand-canonical ensemble (global conservation laws)
  Jeon, Koch, PRL ’00; Bzdak, Skokov, Koch, PRC ’13;
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**Canonical vs grand-canonical**

**Grand-canonical ensemble:** the system exchanges conserved charges with a heat bath

**Canonical ensemble:** conserved charges fixed to a same set of values in all microstates

**Thermodynamic equivalence:** in the limit $V \to \infty$ all statistical ensembles are equivalent wrt to all average quantities, e.g. $\langle N \rangle_{GCE} = N_{CE}$
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**Thermodynamic equivalence:** in the limit $V \to \infty$ all statistical ensembles are equivalent wrt to all average quantities, e.g. $\langle N \rangle_{GCE} = N_{CE}$

Thermodynamic equivalence does *not* extend to fluctuations. The results are ensemble-dependent in the limit $V \to \infty$

So what ensemble should one use?

Canonical? Grand-canonical? Something else?

Begun, Gorenstein, Gazdzicki, Zozulya, PRC ‘04
Applicability of the GCE in heavy-ion collisions

Experiments measure fluctuations in a finite momentum acceptance

\[ \Delta Y_{total} \gg \Delta Y_{accept} \gg \Delta Y_{kick}, \Delta Y_{corr} \] and momentum-space correlation is strong (e.g. Bjorken flow)

In practice difficult to satisfy all conditions simultaneously

**This talk:** \( \Delta Y_{total} \gg \Delta Y_{accept} \rightarrow \Delta Y_{total} > \Delta Y_{accept} \) for any equation of state
Subensemble acceptance method (SAM)

Partition a thermal system with a globally conserved charge $B$ (*canonical ensemble*) into two subsystems which can exchange the charge $V_1 + V_2 = V$

Assume thermodynamic limit:

$$V, V_1, V_2 \to \infty; \quad \frac{V_1}{V} = \alpha = \text{const}; \quad \frac{V_2}{V} = (1 - \alpha) = \text{const};$$

$$V_1, V_2 \gg \xi^3, \quad \xi = \text{correlation length}$$

The canonical partition function then reads:

$$Z_{\text{ce}}(T, V, B) = \text{Tr} \ e^{-\beta \hat{H}} \approx \sum_{B_1} Z_{\text{ce}}(T, V_1, B_1) Z_{\text{ce}}(T, V - V_1, B - B_1)$$

The probability to have charge $B_1$ is:

$$P(B_1) \propto Z_{\text{ce}}(T, \alpha V, B_1) Z_{\text{ce}}(T, (1 - \alpha)V, B - B_1), \quad \alpha \equiv V_1/V$$

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905
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Textbook: $\alpha \rightarrow 0 \implies \text{grand-canonical ensemble} \neq \text{SAM: } 0 < \alpha < 1$

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905
Subensemble acceptance method (SAM)

In the thermodynamic limit, $V \to \infty$, $Z^{ce}$ expressed through free energy density

$$Z^{ce}(T, V, B) \overset{V \to \infty}{=} \exp \left[- \frac{V}{T} f(T, \rho_B) \right]$$

Cumulant generating function for $B_1$:

$$G_{B_1}(t) \equiv \ln \langle e^t B_1 \rangle = \ln \left\{ \sum_{B_1} e^t B_1 \exp \left[- \frac{\alpha V}{T} f(T, \rho_{B_1}) \right] \exp \left[- \frac{\beta V}{T} f(T, \rho_{B_2}) \right] \right\} + \tilde{C}$$

Cumulants of $B_1$:

$$\kappa_n[B_1] = \left. \frac{\partial^n G_{B_1}(t)}{\partial t^n} \right|_{t=0} \equiv \tilde{\kappa}_n[B_1(t)] \quad \text{or} \quad \kappa_n[B_1] = \left. \frac{\partial^{n-1} \tilde{\kappa}_1[B_1(t)]}{\partial t^{n-1}} \right|_{t=0}$$

All $\kappa_n$ can be calculated by determining the $t$-dependent first cumulant $\tilde{\kappa}_1[B_1(t)]$
Subensemble acceptance method (SAM)

\[ \tilde{\kappa}_1[B_1(t)] = \frac{\sum_{B_1} B_1 \tilde{P}(B_1; t)}{\sum_{B_1} \tilde{P}(B_1; t)} \equiv \langle B_1(t) \rangle \quad \text{with} \quad \tilde{P}(B_1; t) = \exp \left\{ tB_1 - V \frac{\alpha f(T, \rho_{B_1}) + \beta f(T, \rho_{B_2})}{T} \right\}. \]

Thermodynamic limit: \( \tilde{P}(B_1; t) \) highly peaked at \( \langle B_1(t) \rangle \)

\( \langle B_1(t) \rangle \) is a solution to equation \( d\tilde{P}/dB_1 = 0 \):

\[ t = \hat{\mu}_B[T, \rho_{B_1}(t)] - \hat{\mu}_B[T, \rho_{B_2}(t)] \]

where \( \hat{\mu}_B \equiv \mu_B/T \), \( \mu_B(T, \rho_B) = \partial f(T, \rho_B)/\partial \rho_B \)

\( t = 0: \rho_{B_1} = \rho_{B_2} = B/V \), \( B_1 = \alpha B \), i.e. conserved charge uniformly distributed between the two subsystems

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905
SAM: Second order cumulant $\kappa_2[B_1]$

\[ t = \hat{\mu}_B[T, \rho_{B_1}(t)] - \hat{\mu}_B[T, \rho_{B_2}(t)] \]

(\*)

\[
\frac{\partial (\ast)}{\partial t} : \quad 1 = \left( \frac{\partial \hat{\mu}_B}{\partial \rho_{B_1}} \right)_T \left( \frac{\partial \rho_{B_1}}{\partial \langle B_1 \rangle} \right)_V \frac{\partial \langle B_1 \rangle}{\partial t} - \left( \frac{\partial \hat{\mu}_B}{\partial \rho_{B_2}} \right)_T \left( \frac{\partial \rho_{B_2}}{\partial \langle B_2 \rangle} \right)_V \frac{\partial \langle B_2 \rangle}{\partial \langle B_1 \rangle} \frac{\partial \langle B_1 \rangle}{\partial t}
\]

\[
\left( \frac{\partial \hat{\mu}_B}{\partial \rho_{B_{1,2}}} \right)_T \equiv \left[ \chi^B_2 (T, \rho_{B_{1,2}}) T^3 \right]^{-1}, \quad \rho_{B_1} \equiv \frac{\langle B_1 \rangle}{\alpha V}, \quad \rho_{B_2} \equiv \frac{\langle B_2 \rangle}{(1 - \alpha) V}, \quad \langle B_2 \rangle = B - \langle B_1 \rangle, \quad \frac{\partial \langle B_1 \rangle}{\partial t} \equiv \tilde{\kappa}_2[B_1(t)]
\]

Solve the equation for $\tilde{\kappa}_2$:

\[
\tilde{\kappa}_2[B_1(t)] = \frac{V T^3}{[\alpha \chi^B_2(T, \rho_{B_1})]^{-1} + [(1 - \alpha) \chi^B_2(T, \rho_{B_2})]^{-1}}
\]

$t = 0$:

\[
\kappa_2[B_1] = \alpha (1 - \alpha) V T^3 \chi^B_2
\]

Higher-order cumulants: iteratively differentiate $\tilde{\kappa}_2$ w.r.t. $t$
SAM: Full result up to $\kappa_6$

\begin{align*}
\kappa_1[B_1] &= \alpha VT^3 \chi_1^B \\
\kappa_2[B_1] &= \alpha VT^3 \beta \chi_2^B \\
\kappa_3[B_1] &= \alpha VT^3 \beta (1 - 2\alpha) \chi_3^B \\
\kappa_4[B_1] &= \alpha VT^3 \beta \left[ \chi_4^B - 3\alpha\beta \frac{(\chi_3^B)^2 + \chi_2^B \chi_4^B}{\chi_2^B} \right] \\
\kappa_5[B_1] &= \alpha VT^3 \beta (1 - 2\alpha) \left\{ [1 - 2\beta\alpha] \chi_5^B - 10\alpha\beta \frac{\chi_3^B \chi_4^B}{\chi_2^B} \right\} \\
\kappa_6[B_1] &= \alpha VT^3 \beta [1 - 5\alpha\beta(1 - \alpha\beta)] \chi_6^B + 5 VT^3 \alpha^2 \beta^2 \left\{ 9\alpha\beta \frac{(\chi_3^B)^2 \chi_4^B}{(\chi_2^B)^2} - 3\alpha\beta \frac{(\chi_3^B)^4}{(\chi_2^B)^3} \\
&\quad - 2(1 - 2\alpha)^2 \frac{(\chi_4^B)^2}{\chi_2^B} - 3[1 - 3\beta\alpha] \frac{\chi_3^B \chi_5^B}{\chi_2^B} \right\}
\end{align*}

$$\beta = 1 - \alpha$$

$$\chi_n^B = \frac{\partial^n (p/T^4)}{\partial(\mu_B/T)^n}$$ — grand-canonical susceptibilities, e.g. from lattice QCD.

Details: V.V., Savchuk, Pobereznyuk, Gorenstein, Koch, 2003.13905
Some common cumulant ratios:

scaled variance

\[
\frac{\kappa_2[B_1]}{\kappa_1[B_1]} = (1 - \alpha) \frac{\chi_2^B}{\chi_1^B},
\]

skewness

\[
\frac{\kappa_3[B_1]}{\kappa_2[B_1]} = (1 - 2\alpha) \frac{\chi_3^B}{\chi_2^B},
\]

kurtosis

\[
\frac{\kappa_4[B_1]}{\kappa_2[B_1]} = (1 - 3\alpha\beta) \frac{\chi_4^B}{\chi_2^B} - 3\alpha\beta \left( \frac{\chi_3^B}{\chi_2^B} \right)^2.
\]

- Global conservation \((\alpha)\) and equation of state \((\chi_n^B)\) effects factorize in cumulants up to the \(3^{rd}\) order, starting from \(\kappa_4\) not anymore
- \(\alpha \to 0\) – GCE limit*
- \(\alpha \to 1\) – CE limit

*As long as \(V_1 \gg \xi^3\) holds

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905
Subensemble acceptance: ideal gas

Ideal gas of baryons and antibaryons: \( \chi_{2n}^B \propto \langle N_B \rangle + \langle N_{\bar{B}} \rangle \), \( \chi_{2n-1}^B \propto \langle N_B \rangle - \langle N_{\bar{B}} \rangle \)

Binomial acceptance \([\text{Bzdak et al., PRC '13}]\)

SAM \([\text{V.V. et al., 2003.13905}]\)

\[
\begin{align*}
\kappa_4/\kappa_2 &\quad - - \quad \kappa_6/\kappa_2 \\
\langle N_B \rangle & = 400, \\
\langle N_{\bar{B}} \rangle & = 100 
\end{align*}
\]

For a more involved test (vdW fluid with a CP) see \(\text{R. Poberezhnyuk, et al., 2004.14358}\)
Net baryon fluctuations at LHC ($\mu_B = 0$)

$$\left( \frac{\kappa_4}{\kappa_2} \right)_{LHC} = (1 - 3\alpha\beta) \frac{\chi_4^B}{\chi_2^B}$$

$$\left( \frac{\kappa_6}{\kappa_2} \right)_{LHC} = [1 - 5\alpha\beta(1 - \alpha\beta)] \frac{\chi_6^B}{\chi_2^B} - 10\alpha(1 - 2\alpha)^2\beta \left( \frac{\chi_4^B}{\chi_2^B} \right)^2$$

For $\alpha > 0.2$ difficult to distinguish effects of the EoS and baryon conservation in $\chi_6^B/\chi_2^B$, $\alpha \leq 0.1$ is a sweet spot where measurements are mainly sensitive to the EoS

Estimates: $\alpha \approx 0.1$ corresponds to $\Delta Y_{acc} \approx 2(1)$ at LHC (RHIC), $p_T$ integrated

V.V., Savchuk, Poberezhnyuk, Gorenstein, Koch, 2003.13905

Lattice data for $\chi_4^B/\chi_2^B$ and $\chi_6^B/\chi_2^B$ from Borsanyi et al., 1805.04445
$\hat{Q}(\hat{Q}_1) \propto Z(T, \alpha V, \hat{Q}_1) Z(T, \beta V, \hat{Q} - \hat{Q}_1)$

**The result:** (see arXiv:2007.03850 for details)

\[
\hat{\kappa}_{i_1}[\hat{Q}^1] = \alpha VT^3 \hat{\chi}_{i_1}, \\
\hat{\kappa}_{i_1i_2}[\hat{Q}^1] = \alpha VT^3 \beta \hat{\chi}_{i_1i_2}, \\
\hat{\kappa}_{i_1i_2i_3}[\hat{Q}^1] = \alpha VT^3 \beta (1 - 2\alpha) \hat{\chi}_{i_1i_2i_3}, \\
\hat{\kappa}_{i_1i_2i_3i_4}[\hat{Q}^1] = \alpha VT^3 \beta \left[(1 - 3\alpha\beta) \hat{\chi}_{i_1i_2i_3i_4} - \frac{\alpha\beta}{2!2!2!} \sum_{\sigma \in S_4} \hat{\kappa}^{-1}_{b_1b_2} \hat{\chi}_{i_\sigma_1i_\sigma_2b_1} \hat{\chi}_{i_\sigma_3i_\sigma_4b_2}\right],
\]

\[\hat{\chi}_{i_1...i_M} = \frac{\partial^M(p/T^4)}{\partial(\mu_{i_1}/T) \ldots \partial(\mu_{i_M}/T)}\]

Results depend on **cross-correlators** of conserved charges

Mathematica notebook to express any $B,Q,S$-cumulant of order $n \leq 6$ in terms of grand-canonical susceptibilities available at [https://github.com/vlvovch/SAM](https://github.com/vlvovch/SAM)

V.V., Poberezhnyuk, Koch, 2007.03850, JHEP ’20
**Key findings:**

- Cumulants up to 3rd order factorize into product of binomial and grand-canonical cumulants

\[
\kappa_{l,m,n} = \kappa_{l+m+n}^{\text{bino}}(\alpha) \times \kappa_{l,m,n}^{\text{gce}}, \quad l + m + n \leq 3
\]

- Ratios of second and third order cumulants are NOT sensitive to charge conservation

- Requires that acceptance fraction \(\alpha\) is the same for all particles

- For order \(n > 3\) charge cumulants “mix”. Effect in HRG is tiny

\[
\kappa_4[B_1^\perp] = \alpha VT^3 \beta \left[ (1 - 3\alpha\beta) \chi_4^B - 3\alpha\beta \frac{(\chi_3^B)^2 \chi_2^Q - 2\chi_{21}^{BQ} \chi_{11}^B \chi_2^B + (\chi_{21}^{BQ})^2 \chi_2^B}{\chi_2^B \chi_2^Q - (\chi_{11}^{BQ})^2} \right].
\]
SAM and non-conserved quantities

\[ \kappa_{XY} = (1 - \alpha) \kappa_{XY}^{gce} + \alpha \kappa_{XY}^{ce} \]

- Mixed cumulants involving one conserved charge e.g. \( pQ \) have \( \kappa_{pQ}^{ce} = 0 \) thus they scale like second order charge cumulants
  - \( p \) and \( Q \), again, must have the same \( a \)
  - STAR tries to measure these [1903.05370]
  - Can ALICE measure them as well?

- Cancellation does NOT occur for two non-conserved quantities, such as \( \kappa_{pK} \)
**Net-proton and net-$\Lambda$ fluctuations**

\[
\kappa_{pp} = (1 - \alpha) \kappa_{pp}^{gce} + \alpha \kappa_{pp}^{ce}
\]

- Allows for corrections due to electric charge (protons) or strangeness ($\Lambda$) conservation in addition to baryon number conservation.

Truth lies in between the “naïve” corrections
Likely bigger effect for higher orders
Net-proton fluctuations at various energies

- **LHC**: The most important (but not the only) effect is **baryon conservation**
- **Low energies**: $\text{net-p} \approx \text{net-Q} \quad \Rightarrow \quad \text{electric charge conservation dominates}$
- **Simultaneous treatment of B and Q conservation** is important
Global conservation effects for pions (kaons) driven by electric charge (strangeness) conservation. Ratios deviate from unity in $\alpha \to 0$ limit due to resonance decays*

*Argument here is made in coordinate space. In momentum space the ratios do tend to unity in limit $\Delta Y_{acc} \to 0$ due to diffusion of decay products in and out of acceptance

Correlations from resonance decays in HRG model included via [Begun et al., PRC '06]
Applicability and limitations

• Argument is based on partition in **coordinate** space but experiments measure in **momentum** space
  • OK at high energies where we have **Bjorken flow**
    • For small \( \Delta Y_{acc} < 1 \): corrections due to thermal smearing and resonance decay kinematics (for Q and S)
  • Limited applicability at lower energies
• **Thermodynamic limit** i.e. \( V_1, V_2 \gg \xi^3 \):
  • OK at LHC where \( \frac{dV}{dy} \sim 4000 - 5000 \text{ fm}^3 \) vs. \( V_{lattice} \sim 125 \text{ fm}^3 \)
    • Applicability is more limited near the critical point
• Assumes \( T, \mu_B = \text{const} \) everywhere
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Address these issues with Monte Carlo SAM Sampler

V.V., V. Koch, to appear
SAM Sampler

A particlization routine that preserves correlations and fluctuations locally

\[
\begin{align*}
T_1, \mu_1, V_1 & \quad T_2, \mu_2, V_2 & \quad \ldots & \quad T_N, \mu_N, V_N \\
\Delta \eta_1 & \quad \Delta \eta_2 & & \quad \Delta \eta_N
\end{align*}
\]

1. Partition the hydro (blast-wave) hypersurface into subvolumes along the space-time rapidity axis such that each \( V_i \gg \xi^3 \) and \( \Delta \eta \leq \Delta Y_{acc} \)
2. Sample each subvolume grand-canonical, using the partition function of an interacting HRG
3. Reject the event if global conservation is violated
4. Sample the momenta of particles
5. Do resonance decays or plug into hadronic afterburner

\( \checkmark \) (event-by-event) hydro
\( \checkmark \) local correlations
\( \checkmark \) global conservation
\( \checkmark \) thermal smearing
\( \checkmark \) resonance decays

To be part of FIST-2.0
A case study: net baryon fluctuations at $\mu_B = 0$

Model the deviations of the lattice data from Skellam distribution at $T_{pc}$ with excluded-volume interactions in the baryonic sector (EV-HRG model)

$$P(N) \sim \frac{(V - bN)^N}{N!} \theta(V - bN)$$

Multiplicity distribution of the EV-HRG model is efficiently sampled with Poisson + rejection sampling
details in V.V., Gorenstein, Stoecker, 1805.01402
A case study: net baryon fluctuations at $\mu_B = 0$

Take only protons and neutrons, $T=160$ MeV, blast-wave momentum smearing

$$\frac{\chi_2^B}{\chi_{2,Sk}^B} = 0.94, \quad \frac{\chi_4^B}{\chi_2^B} = 0.69, \quad \frac{\chi_6^B}{\chi_2^B} = -0.18 \quad \leftarrow \text{compatible with lattice}$$

boost-invariant, $\Delta \eta = 0.1$, $\eta_{\text{max}} = \pm 5$, $V_i = 20$ fm$^3$, baryon number conservation only
A case study: net baryon fluctuations at $\mu_B = 0$

- Thermal smearing “poissonizes” fluctuations in small acceptance
- The signal survives for sufficiently large rapidity coverage, $\Delta Y_{acc} \gtrsim 1$
• net proton ≠ net baryon

• net proton kurtosis crosses the GCE/LQCD value of net baryon kurtosis in certain rapidity range ($\Delta Y_{acc} \sim 1 - 2$) → explanation for apparent agreement between STAR and LQCD reported in [HotQCD, 2001.08530]?
Summary

• SAM is a method to correct cumulants of distributions in heavy-ion collisions for global (multiple) charge conservation for any equation of state, not just ideal gas
  
  • connection to lattice results

  • ratios of second and third order cumulants insensitive to conservation effects as long as acceptance fraction is the same

  • electric charge and strangeness conservations affect net-proton and net-$\Lambda$ fluctuations in addition to baryon number conservation

• SAM sampler is a particlization routine for quantitative analysis of event-by-event fluctuations
Summary

• SAM is a method to correct cumulants of distributions in heavy-ion collisions for global (multiple) charge conservation for any equation of state, not just ideal gas
  - connection to lattice results
  - ratios of second and third order cumulants insensitive to conservation effects as long as acceptance fraction is the same
  - electric charge and strangeness conservations affect net-proton and net-Λ fluctuations in addition to baryon number conservation

• SAM sampler is a particlization routine for quantitative analysis of event-by-event fluctuations

Thanks for your attention!
Backup slides
**Binomial acceptance vs actual acceptance**

*Binomial acceptance:* accept each particle (charge) with a probability $\alpha$ independently from all other particles.

**SAM:**
Subensemble acceptance: van der Waals fluid

van der Waals equation of state: first-order phase transition and a critical point

\[ Z_{\text{vdW}}^{\text{ce}}(T, V, N) = Z_{\text{id}}^{\text{ce}}(T, V - bN, N) \exp \left( \frac{aN^2}{VT} \right) \theta(V - bN) \]

Rich structures in cumulant ratios close to the CP

V.V., Poberezhnyuk, Anchishkin, Gorenstein, 1507.06537
Subensemble acceptance: van der Waals fluid

Calculate cumulants $\kappa_n[N]$ in a subvolume directly from the partition function

$$P(N) \propto Z_{vdW}^c(T, xV_0, N) Z_{vdW}^c(T, (1-x)V_0, N_0 - N)$$

and compare with the subensemble acceptance results

Results agree with subensemble acceptance in thermodynamic limit ($N_0 \to \infty$)

Finite size effects are strong near the critical point: a consequence of large correlation length $\xi$

R. Poberezhnyuk, O. Savchuk, et al., 2004.14358