Recent thermal model developments: the The(rmal-)FIST package

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https://github.com/vlvovch/Thermal-FIST

ECT Workshop — Observables of Hadronization and the QCD Phase Diagram in the Cross-over Domain*

Trento, Italy, October 15-19, 2018

FIAS Frankfurt Institute for Advanced Studies

GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Thermal model

$$N_i^{\mathrm{hrg}} = V\frac{d_i m_i^2 T}{2\pi^2} K_2\left(\frac{m_i}{T}\right) e^{\frac{\mu_i}{T}},\ N_i^{\mathrm{tot}} = N_i^{\mathrm{hrg}} + \sum_j BR(j \to i) N_j^{\mathrm{hrg}},\ i \epsilon HRG$$

Common tools: (not an exhaustive list)

1) **SHARE 3** [G. Torrieri, J. Rafelski, M. Petran, et al.]
   Fortran/C++. Chemical (non-)equilibrium, fluctuations, charm, nuclei
   open source: http://www.physics.arizona.edu/~gtshare/SHARE/share.html

2) **THERMUS 4** [S. Wheaton, J. Cleymans, B. Hippolyte, et al.]
   C++/ROOT. Canonical ensemble, EV corrections, charm, nuclei
   open source: https://github.com/thermus-project/THERMUS

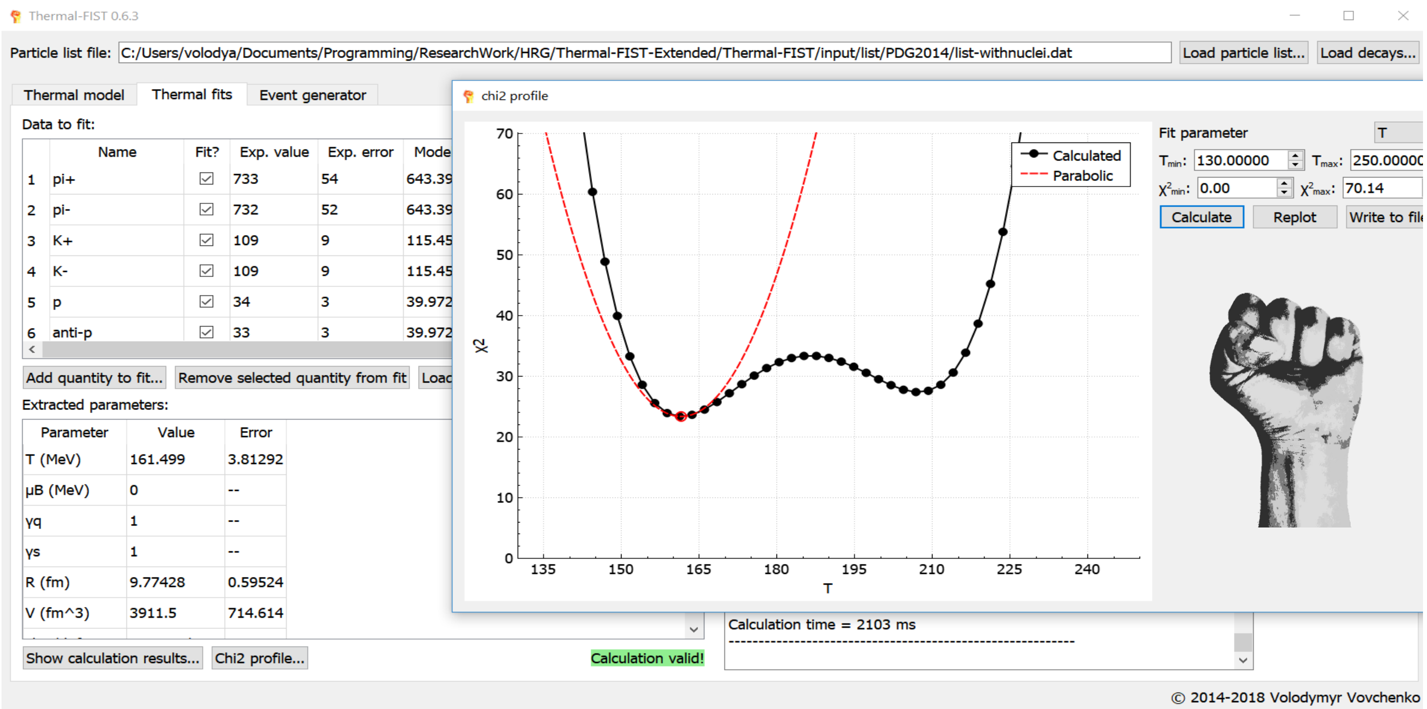
3) **GSI-Heidelberg** code [A. Andronic et al.] **not open source**

4) **Florence** code [F. Becattini et al.] **not open source**

Thermal-FIST [**V.V.**, H. Stoecker; Uni-Frankfurt]

User-friendly thermal model package for *general-purpose applications*

open source **(GPL-3.0, C++):** https://github.com/vlvovch/Thermal-FIST



Thermal-FIST

[**V.V.**, H. Stoecker; Uni-Frankfurt]

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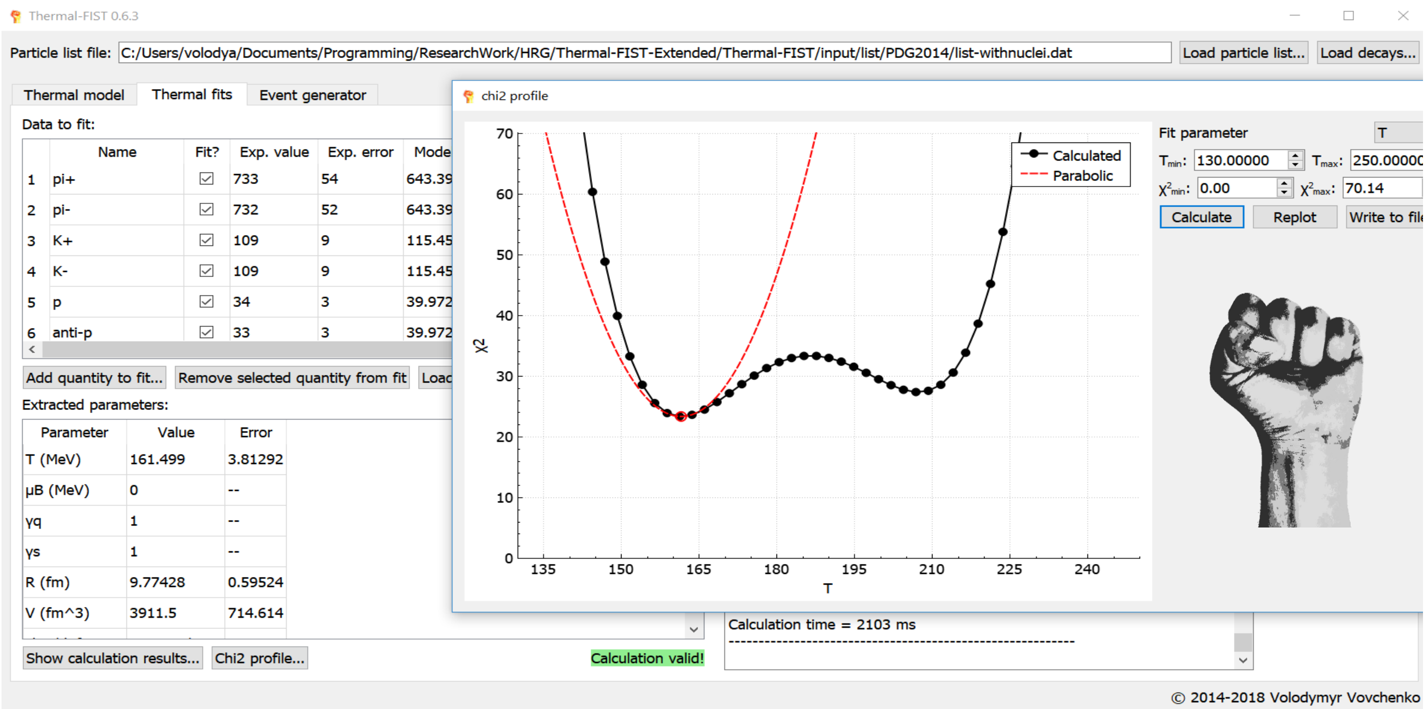


"So that's how you get your results so quickly!"

J. Cleymans

"Thanks for reproducing my results!"

F. Becattini

Thermal model aspects in Thermal-FIST

Alternative/extended scenarios:

- chemical non-equilibrium (γ_q, γ_s)
- **light nuclei**

Equation of state

Extensions of the HRG model:

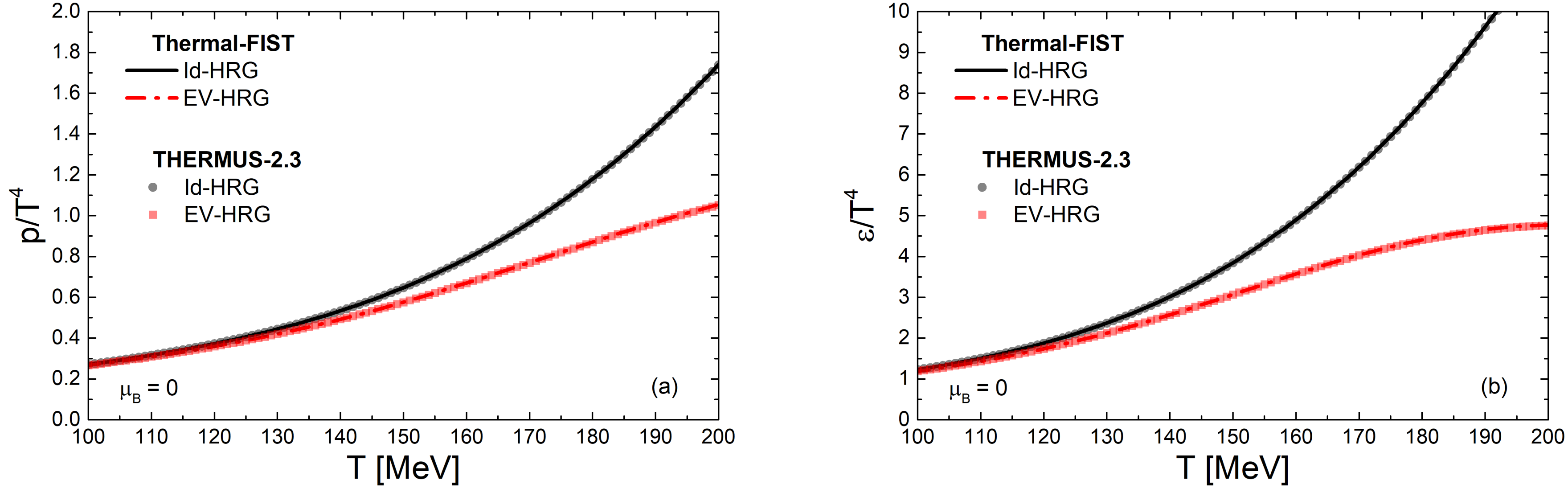
- **different treatment of finite resonance widths**
- **repulsive interactions (excluded volume)**
- van der Waals interactions (*criticality*) **M. Gorenstein, talk Thursday**
- particle number fluctuations and correlations (probabilistic decays, EV/vdW interactions)

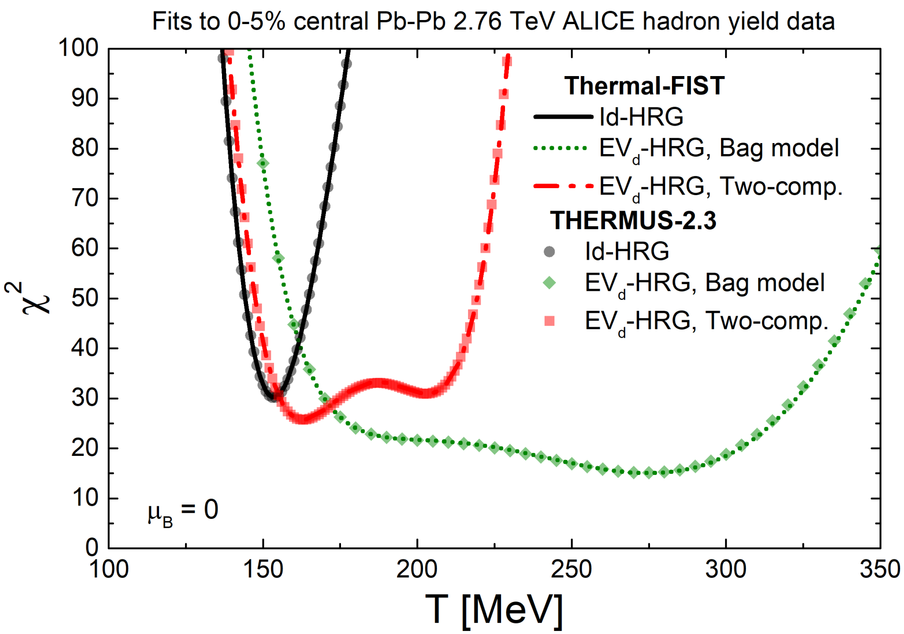
Canonical statistical model (CSM):

- **exact conservation of conserved charges**

Monte Carlo event generator (Blast-wave, CSM, interactions)

FIST in THERMUS mode: cross-check





FIST results coincide with THERMUS, provided that the same input used

Finite resonance widths

resonances have finite lifetime,
their width should be taken into account

Breit-Wigner spectral density usually used in thermal models

[Becattini, ZPC ’96; Torrieri et al. (SHARE); Wheaton et al. (THERMUS); Andronic et al. (GSI-HD), NPA ‘06]

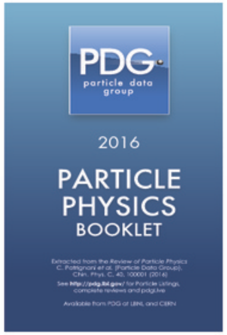
We explore finite widths effects on final hadron yields

V. Vovchenko, M.I. Gorenstein, H. Stoecker, Phys. Rev. C 98, 034906 (2018)

source code: https://github.com/vlvovch/1807.02079

Modeling finite resonance widths

$$n_i(T,\mu;m_i) \to \int_{m_i^{\min}}^{m_i^{\max}} dm\, \rho_i(m)\, n_i(T,\mu;m)$$



Broad Δ and N^* resonances appear in πN scattering…

Use πN scattering phase shifts? $\rho_i(m) \propto \dfrac{\partial \delta_{\pi N}(m)}{\partial m}$

[P.M. Lo, Friman, Redlich, Sasaki, 1710.02711]

- Seems appropriate for $\Delta(1232)$
- Higher-mass resonances mainly have 3-body final states
- S-matrix would require a coupled-channel treatment?

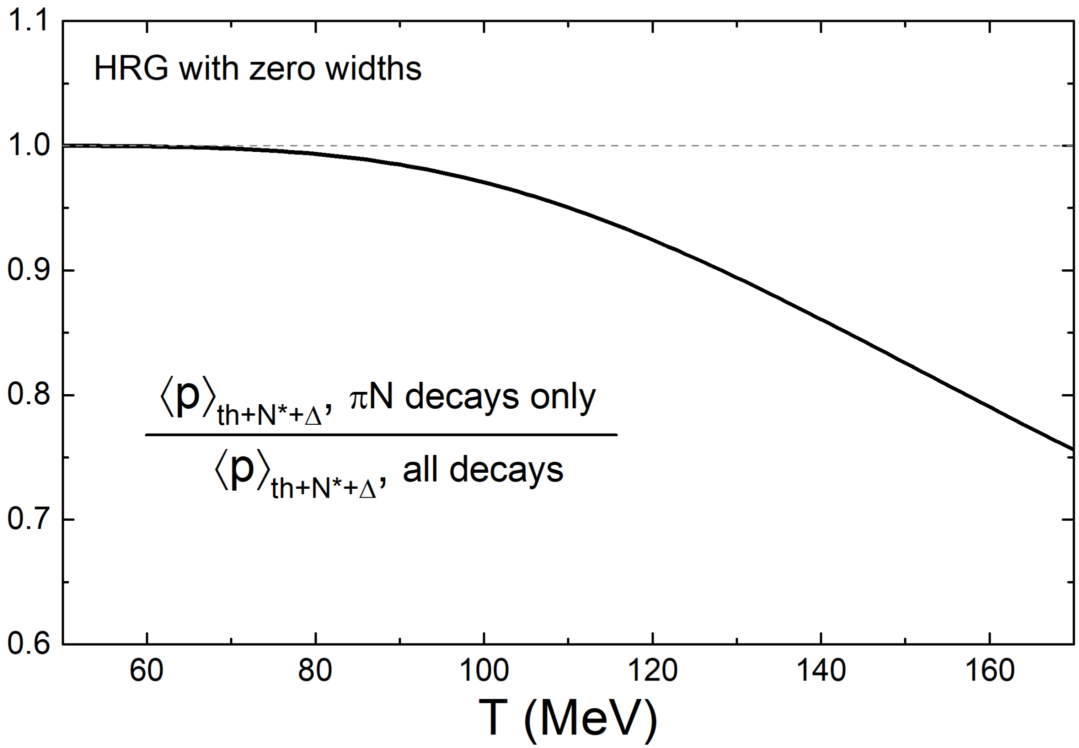
Δ(1600) DECAY MODES	Fraction (Γ_i/Γ)
$N\pi$	10–25 %
$N\pi\pi$	75–90 %
$\Delta(1232)\pi$	73–83 %
$\Delta(1232)\pi$, P-wave	72–82 %
$\Delta(1232)\pi$, F-wave	<2 %
$N(1440)\pi$, P-wave	seen

Δ(1620) DECAY MODES	Fraction (Γ_i/Γ)
$N\pi$	20–30 %
$N\pi\pi$	55–80 %

To what extent can πN channels describe Δ's and N^*'s?

πN channels for Δ and N^*

Δ and N^* proton feeddown through πN only vs the full feeddown,
i.e. throw away protons from e.g. $\Delta, N^* \rightarrow p\pi\pi$ decays



- Suppression of proton yield at high T if only πN decays taken
- Would describe, but *not* explain, the 'proton anomaly'

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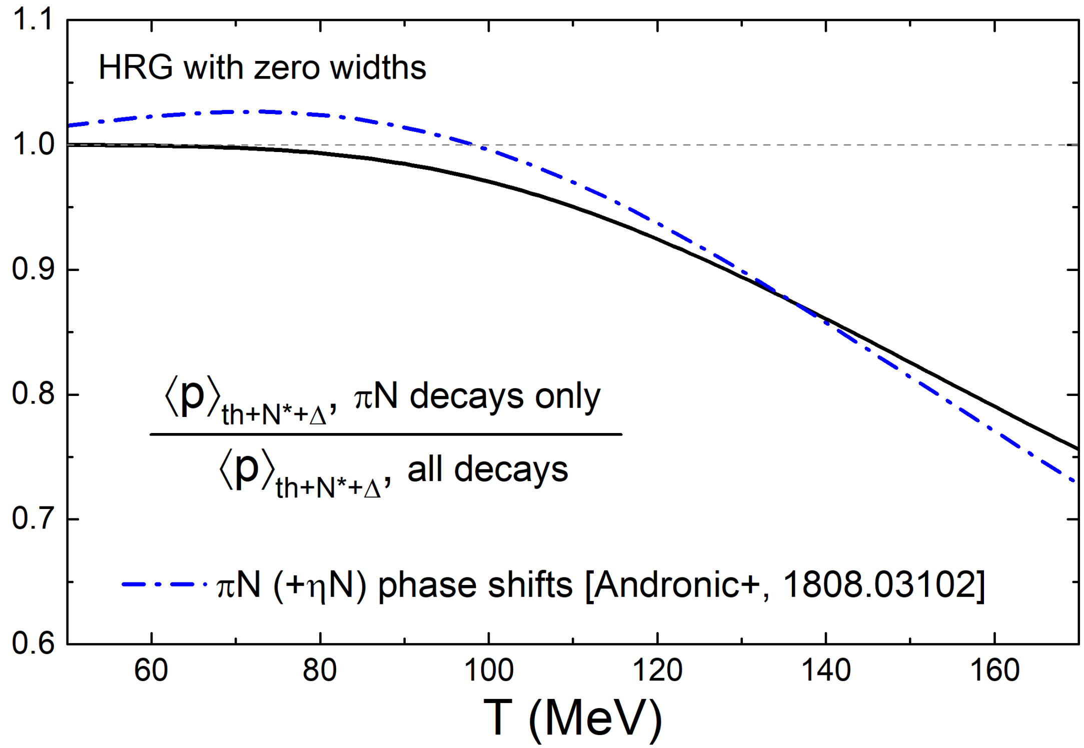


- Suppression of proton yield at high T if only πN decays taken
- Would describe, but *not* explain, the 'proton anomaly'
- Similar *p* suppression in phase shift calculation [Andronic et al., 1808.03102]

Different scenarios for spectral functions

More conservative approach: consider different prescriptions to estimate the systematic error coming from resonance widths modeling

Thermal-FIST implements three options:

1) Zero-width approximation $\rho_i(m) = \delta(m - m_i)$

Simplest possibility, used commonly in LQCD comparisons

2) Fixed Breit-Wigner (BW) in $\pm 2\Gamma_i$ interval $\rho_i(m) = A_i \frac{2\, m\, m_i\, \Gamma_i}{(m^2 - m_i^2)^2 + m_i^2\, \Gamma_i^2}$

Popular choice in thermal fits (e.g. THERMUS), no threshold suppression

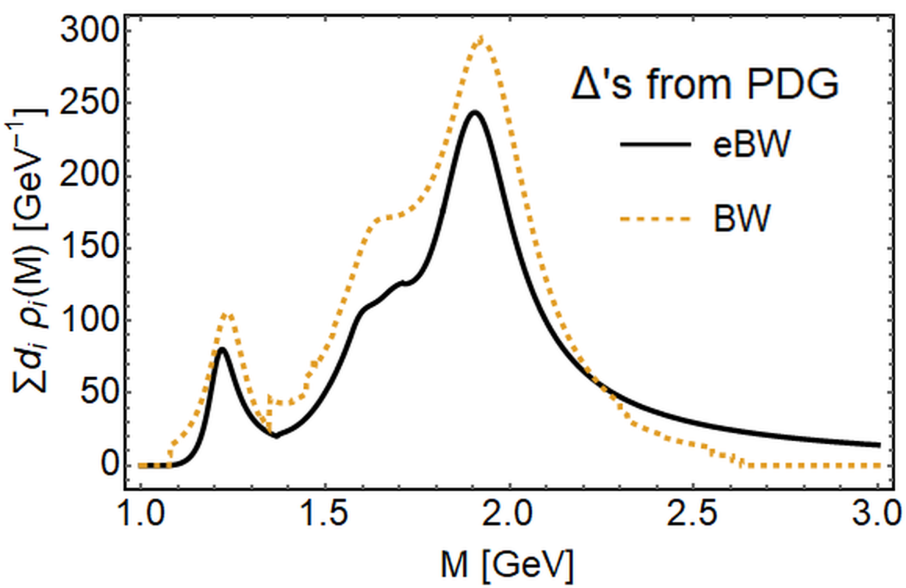
3) Energy-dependent Breit-Wigner (eBW) $\Gamma_i(m) = \sum_j \Gamma_{i\to j}(m)$

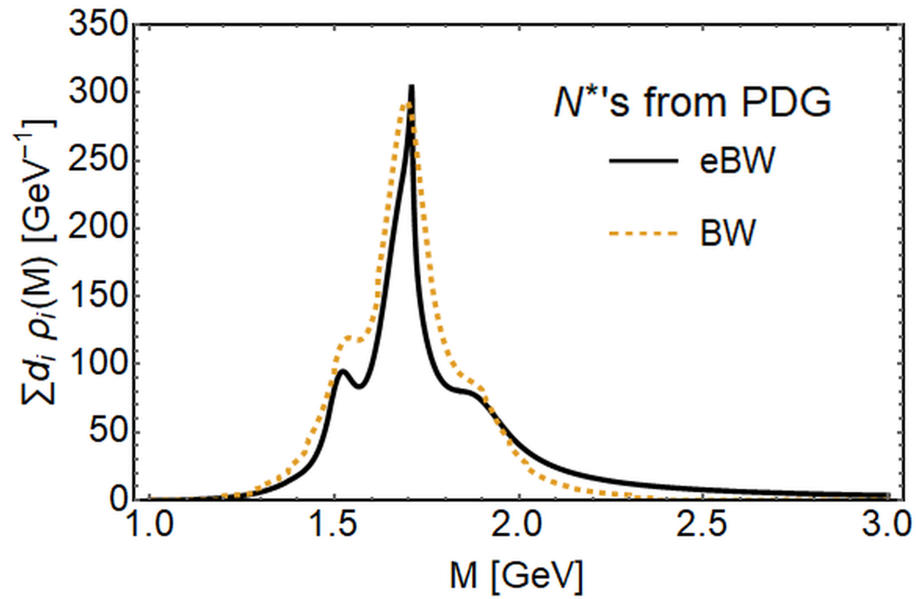
$$\Gamma_{i\to j}(m) = b_{i\to j}^{pdg}\, \Gamma_i^{pdg} \left[1 - \left(\frac{m_{i\to j}^{thr}}{m}\right)^2\right]^{l_{ij}+1/2}$$

suppression at threshold

+ m-dependent decay feeddown $N_i^{tot} = N_i^{hrg} + \sum_{j\in pdg} \int dm\, BR(j \to i; m)\, \rho_j(m)\, N_j^{hrg}(m)$

Modeling widths: Spectral functions

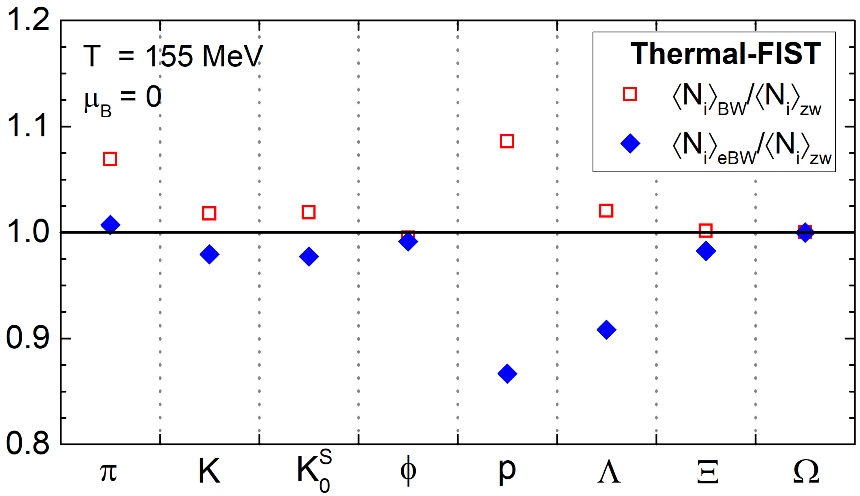


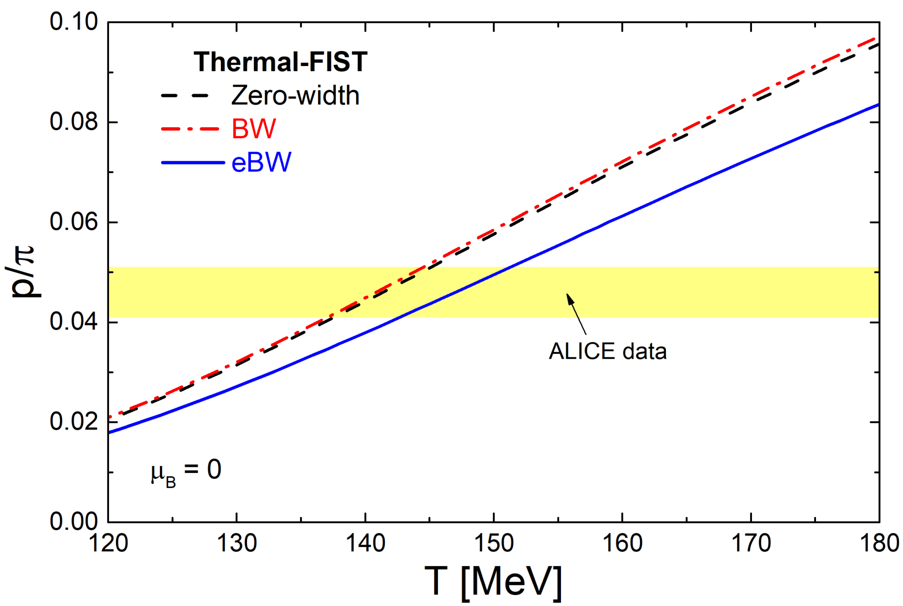


- **BW:** spectral function shifted to lower masses
- **eBW:** spectral function shifted to higher masses
- Overall normalization same, but difference shows up in thermodynamics due to integration with the Boltzmann factor

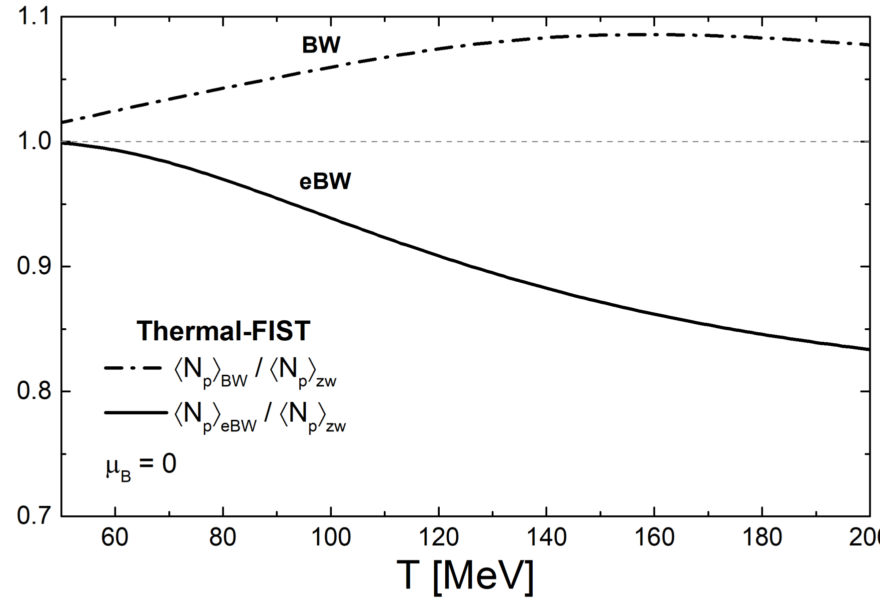
Modeling widths: Effect on hadron yields

Modification of final hadron yields



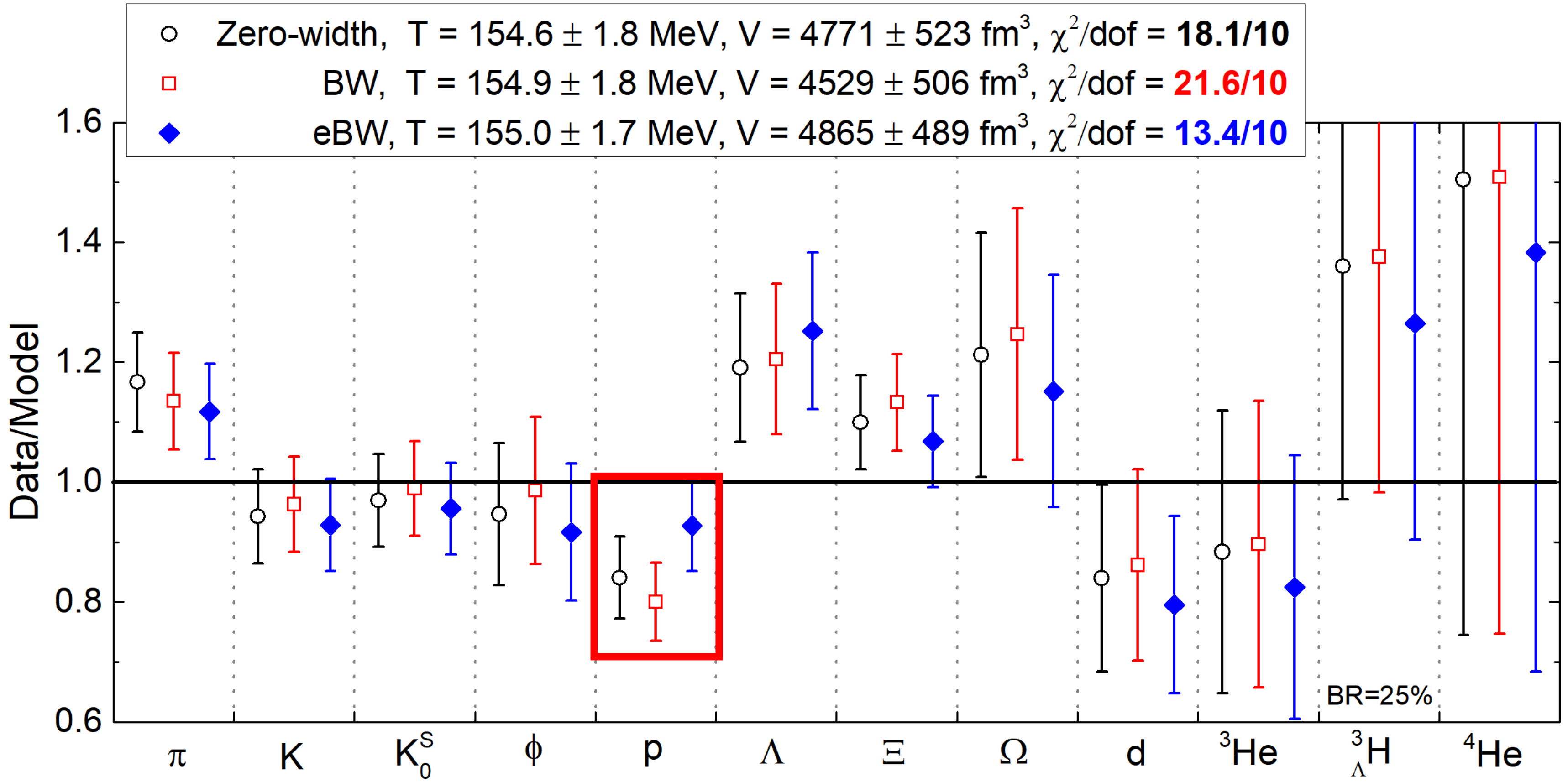


protons



- BW enhances, eBW suppresses feeddown
- Strongest effect for protons & Λ
- p/π ratio suppressed in eBW

Modeling widths: Thermal fits at LHC



- **'Proton anomaly' largely eliminated in the eBW scheme**
- **Systematic uncertainties due to widths modeling are significant**
- **Outlook:** combine with other effects (excluded volume, non-eq.,…)

Modeling widths: Thermal fits at RHIC

0-5% STAR BES data (π, K, p, Λ, Ξ), weak decay feeddown for protons incl.

Q/B = 0.4, S = 0 $\rightarrow$ μ_Q, μ_S [STAR collaboration, 1808.03102]

$\sqrt{s_{NN}}$ (GeV)	Scheme	Fit results		
		T (MeV)	μ_B (MeV)	χ^2/dof
7.7	zero-width	144.3 ± 2.5	417 ± 15	$13.9/7$
	BW	144.3 ± 2.5	415 ± 15	$15.6/7$
	eBW	146.9 ± 2.7	427 ± 17	$10.8/7$
11.5	zero-width	153.1 ± 2.8	303 ± 14	$9.2/7$
	BW	153.4 ± 2.8	303 ± 14	$10.4/7$
	eBW	155.4 ± 2.8	309 ± 15	$5.5/7$
19.6	zero-width	159.2 ± 3.3	199 ± 12	$14.5/7$
	BW	159.4 ± 3.3	199 ± 12	$16.5/7$
	eBW	162.0 ± 3.4	203 ± 13	$8.8/7$
27	zero-width	161.0 ± 3.3	156 ± 11	$15.5/7$
	BW	161.1 ± 3.3	156 ± 11	$18.0/7$
	eBW	164.1 ± 3.4	159 ± 11	$9.0/7$
39	zero-width	161.5 ± 3.1	106 ± 10	$14.0/7$
	BW	161.4 ± 3.1	106 ± 10	$16.4/7$
	eBW	164.6 ± 3.2	109 ± 10	$8.0/7$

Small systems and canonical ensemble

thermal model applied also for small systems, even for elementary reactions like $e^+e^-, pp, p\bar{p}$

[Becattini et al., ZPC '95, ZPC '97]

canonical treatment of (some) conserved charges needed when the reaction volume is small, suppresses yields

[Rafelski, Danos, et al., PLB '80]

Here applications to LHC data are considered

V. Vovchenko, B. Doenigus, H. Stoecker, Phys. Lett. B 785, 171 (2018), work in progress

Canonical statistical model (CSM)

Canonical partition function: [Becattini et al., ZPC ‘95, ZPC ‘97]

$$\mathcal{Z}(B,Q,S) = \int_{-\pi}^{\pi} \frac{d\phi_B}{2\pi} \int_{-\pi}^{\pi} \frac{d\phi_Q}{2\pi} \int_{-\pi}^{\pi} \frac{d\phi_S}{2\pi} \, e^{-i\,(B\phi_B + Q\phi_Q + S\phi_S)} \exp\left[\sum_j z_j^1 \, e^{i\,(B_j\phi_B + Q_j\phi_Q + S_j\phi_S)}\right]$$

$$z_j^1 = V_c \int dm \, \rho_j(m) \, d_j \frac{m^2 T}{2\pi^2} K_2(m/T) \qquad \langle N_j^{\rm prim} \rangle^{\rm ce} = \frac{Z(B-B_j, Q-Q_j, S-S_j)}{Z(B,Q,S)} \langle N_j^{\rm prim} \rangle^{\rm gce}$$

chemical factors, ≈ 1 at large volume (GCE)

CSM implementation in Thermal-FIST:

- Selective canonical treatment of charges
- Full quantum statistics
- Supports $|B_j| > 1$ **(light nuclei)**
- Particle number fluctuations and correlations
- EV/vdW interactions within Monte Carlo formulation [**V.V.** et al., 1805.01402]

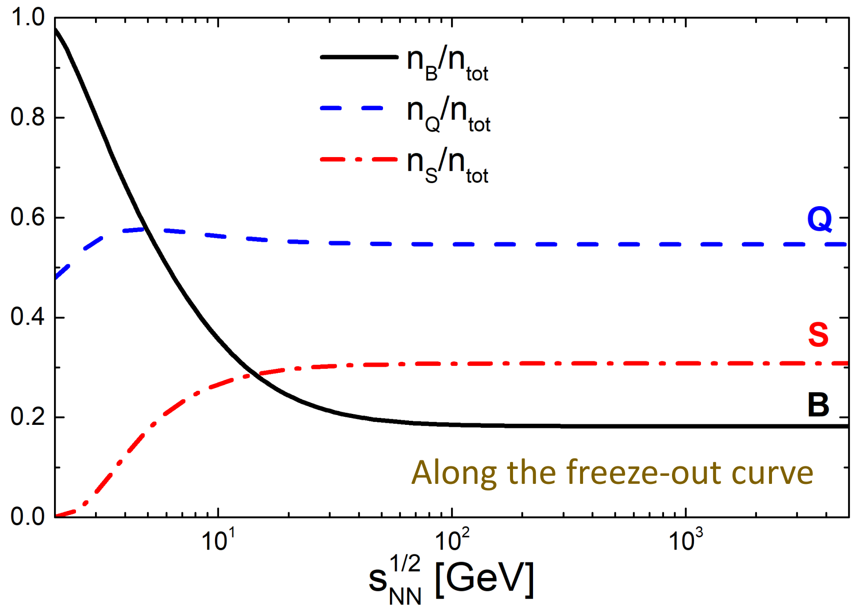
```
model.ConserveBaryonCharge(true);
model.ConserveElectricCharge(false);
model.ConserveStrangeness(true);
```

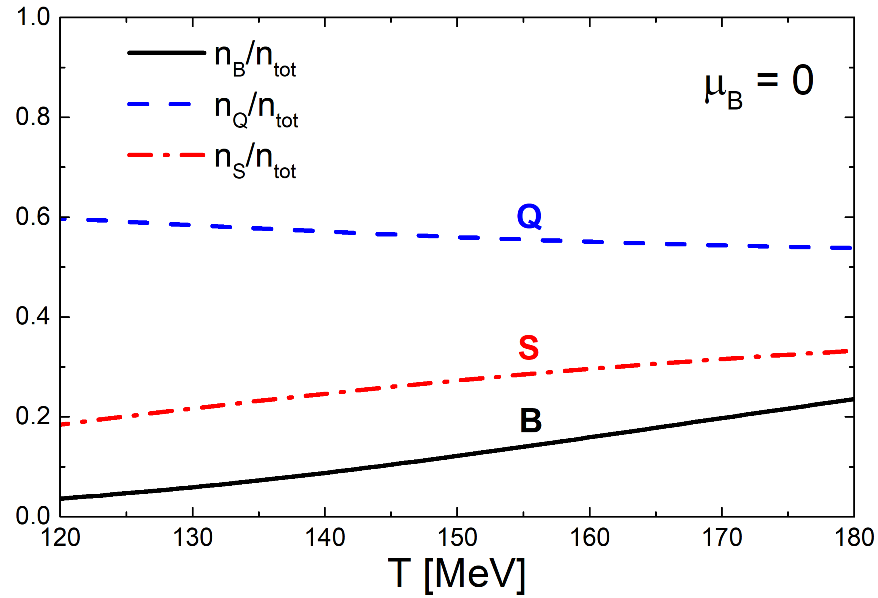
When is the canonical treatment necessary?

Normally, when the total number of particles carrying a conserved charge is smaller or of the order of unity

The canonical treatment is often restricted to strangeness only (SCE)

[STAR collaboration, 1701.07065; ALICE collaboration, 1807.11321]





- **Strangeness** conservation is most important at low energies (**HADES, CBM**)
- *Small systems at **RHIC** and **LHC**:* exact **baryon** conservation at least as important as **strangeness**

CSM at LHC

Enforce exact conservation of charges, $B = Q = S = 0$, in a *correlation volume* V_C around midrapidity

In general, $\boldsymbol{V_C \neq dV/dy}$

Causality argument: exact conservation across a few units of rapidity?

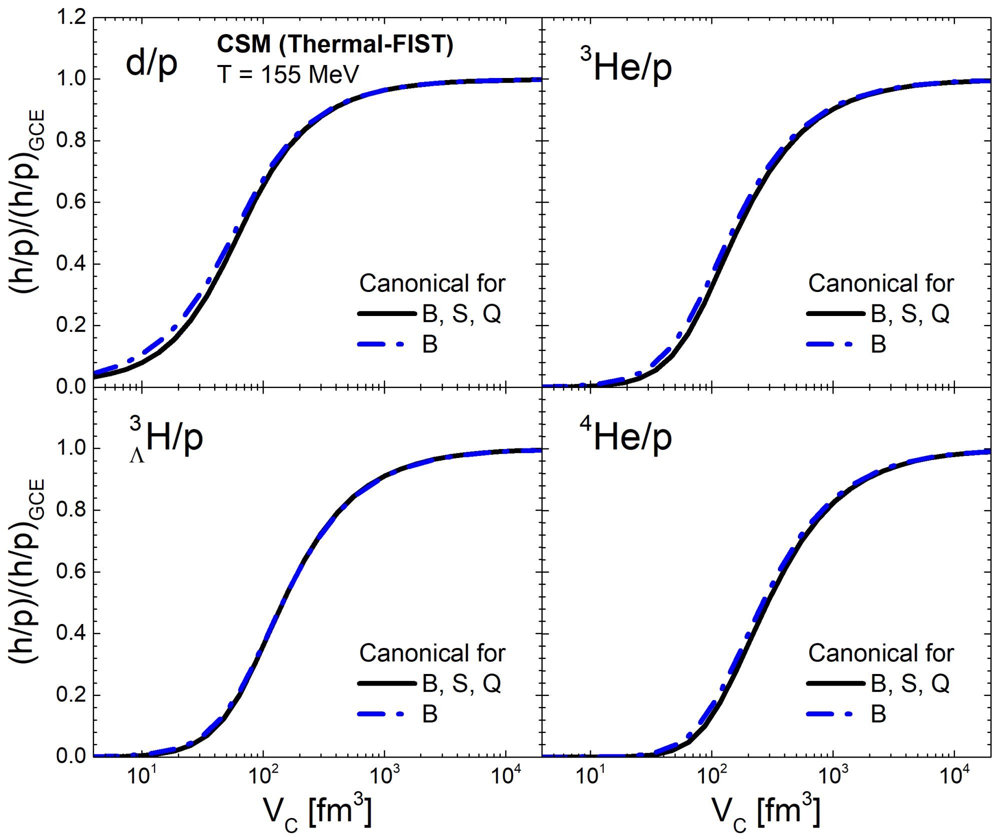
[Castorina, Satz, 1310.6932]

New application:

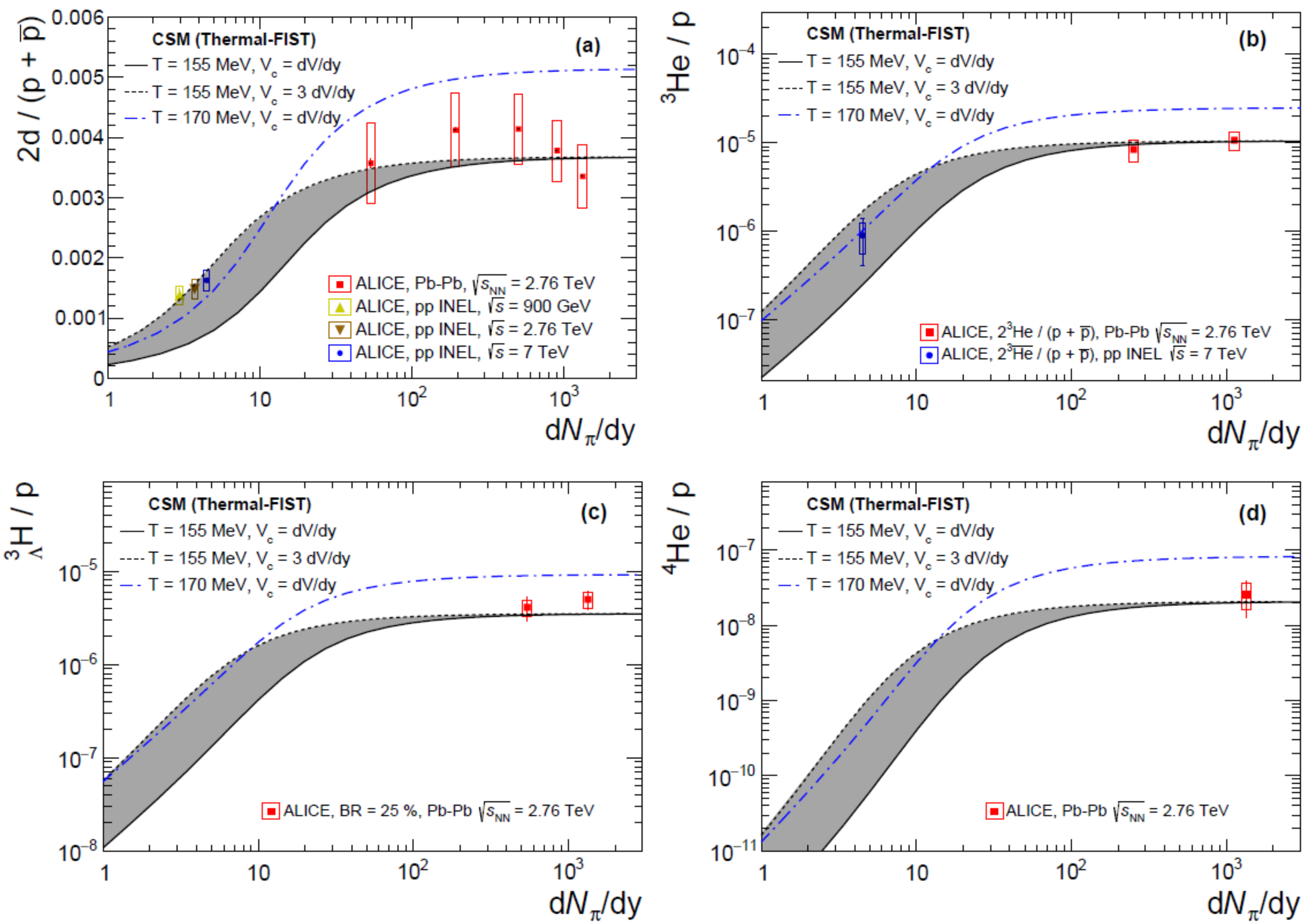
CSM for **light nuclei**

- Suppression of nuclei-to-proton ratios at low multiplicities

- For these observables sufficient to enforce exact baryon conservation only



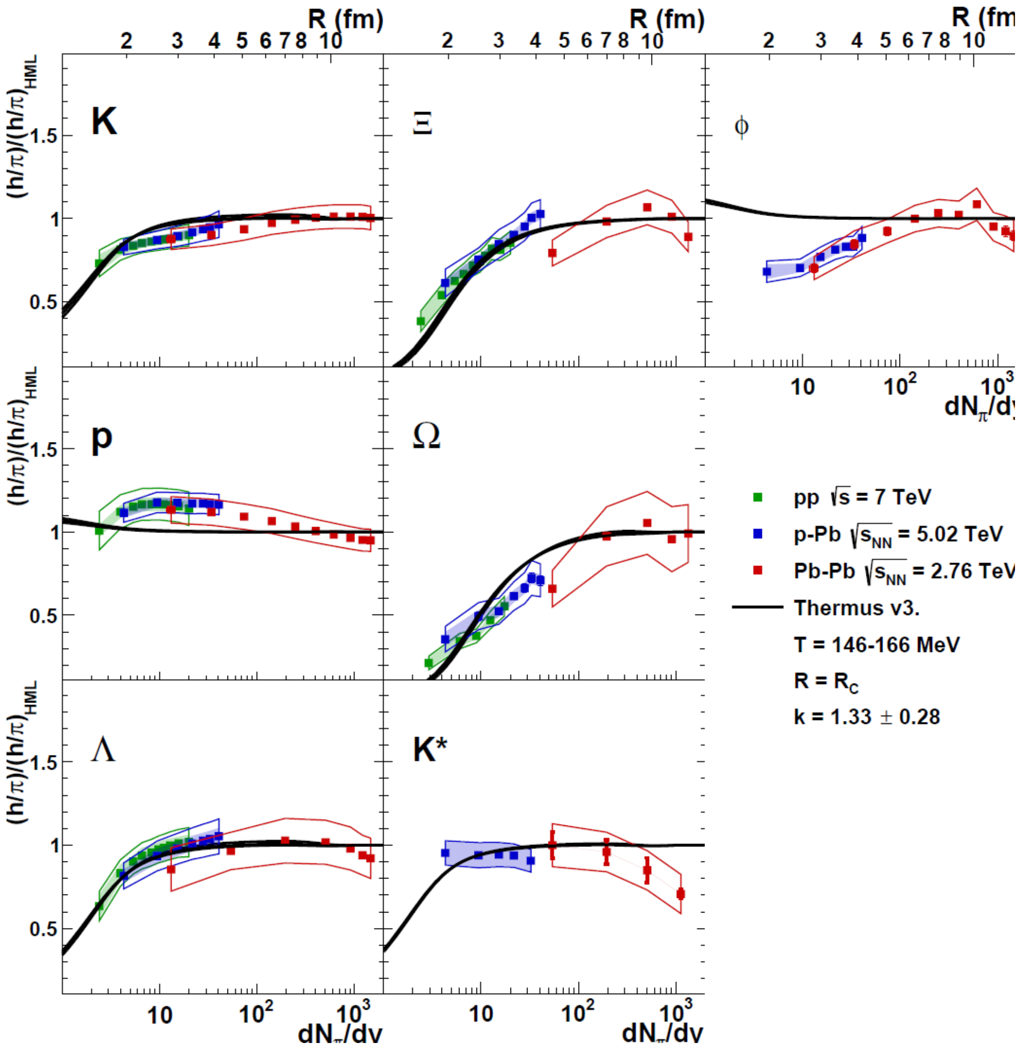
CSM at LHC: light nuclei



[**V.V.**, B. Doenigus, H. Stoecker, 1808.05245]

- **CSM** qualitatively captures the behavior seen in the data
- Data prefers $V_C > dV/dy$ and/or $T_{p+p} > T_{Pb+Pb}$

CSM at LHC: light flavor hadrons

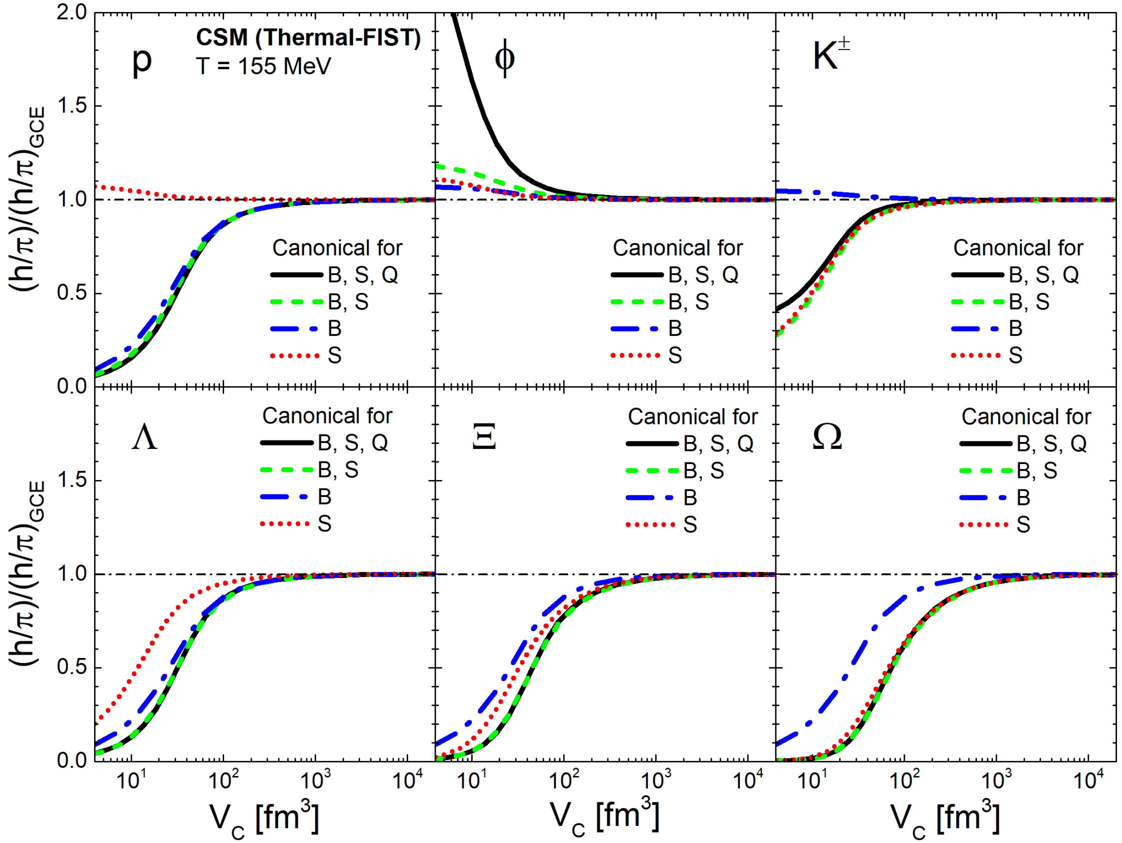


[ALICE collaboration, 1807.11321]

- ALICE data show clear multiplicity dependence
- Have been considered in strangeness-canonical picture only
  [Vislavicius, Kalweit, 1610.03001]
- What is the role of baryon and electric charge conservation?

CSM at LHC: correlation volume dependence

Correlation volume dependence within various mixed-canonical ensembles



[**V.V.**, B. Doenigus, H. Stoecker, in preparation]

- SCE appropriate for K, Ω, Ξ, less for Λ, totally off for p and ϕ
- Baryon-strangeness CE appropriate for most observables, except ϕ/π
- Tension with data for ϕ/π and p/π

CSM at LHC: summary

- Canonical picture seems to work fairly well for strange hadrons and for light nuclei

- ϕ/π and p/π ratios are not described by CSM

- Strangeness-canonical ensemble is only appropriate for charged kaons and multistrange hyperons, exact baryon conservation needed for other observables

- Outlook: Finite-size effects (excluded volume) within CSM, in particular for light nuclei

Excluded volume corrections

Notion that hadrons have finite eigenvolume suggested a while ago

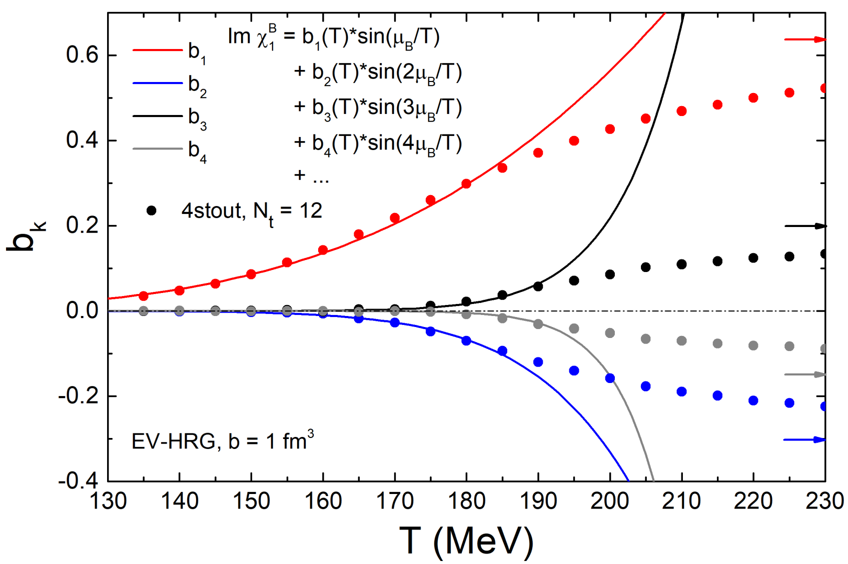
[R. Hagedorn, J. Rafelski, PLB '80]

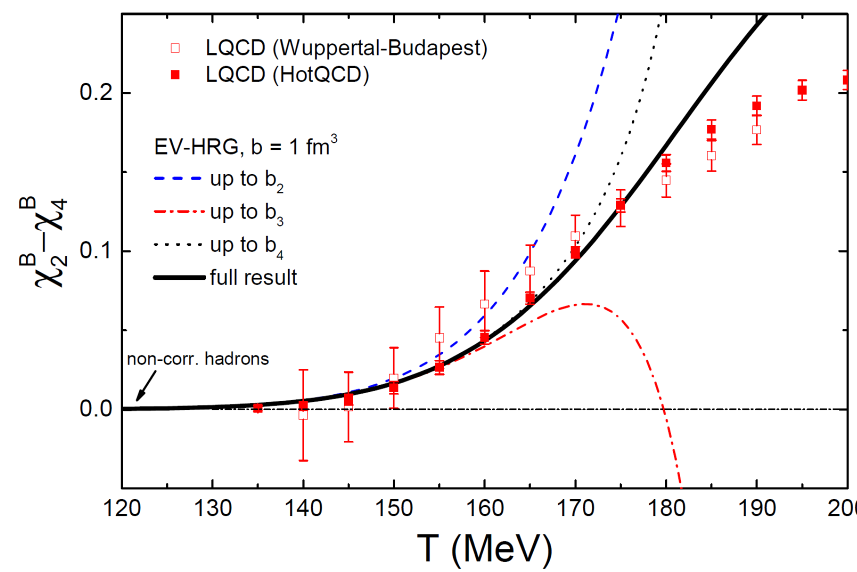
Excluded volume model: $V \to V - bN \quad \Rightarrow$ repulsive interactions

[D. Rischke et al., Z. Phys. C '91]

Whether EV corrections are needed at all has been debated...

Recent lattice data favor EV-like effects in baryonic interactions





V.V., A. Pasztor, Z. Fodor, S.D. Katz, H. Stoecker, 1708.02852

but not much info regarding (non-)existence of EV effects for mesons

“One size fits them all” scenario

EV model: $N_i \propto \exp\left(-v_i \frac{p}{T}\right)$ ← larger hadrons suppressed

EV effects cancel out in hadron yield ratios if $v_i \equiv v$, volume renormalized

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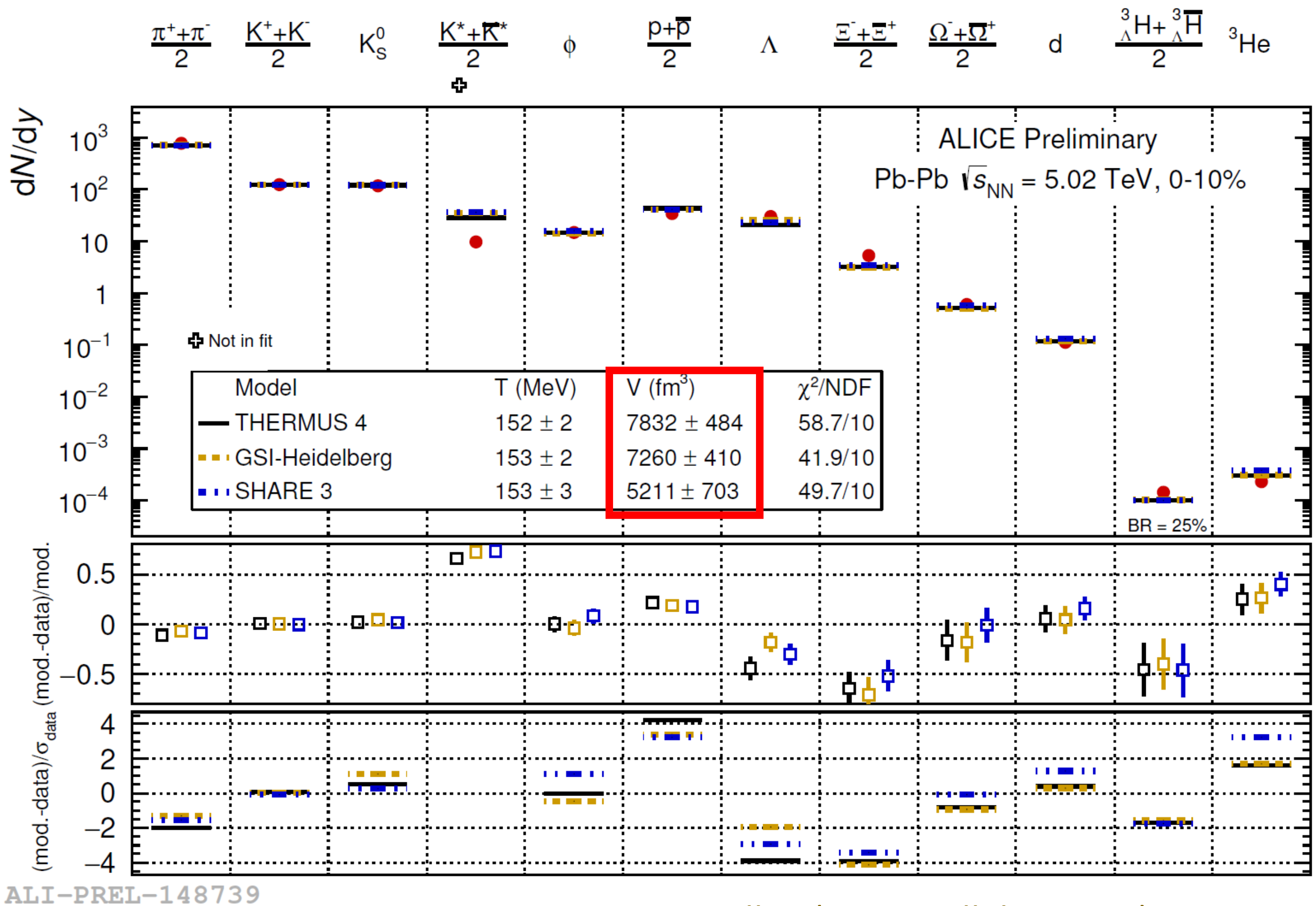


GSI-HD, THERMUS:

$r = 0.3$ fm for *all* mesons, baryons, and *light nuclei*

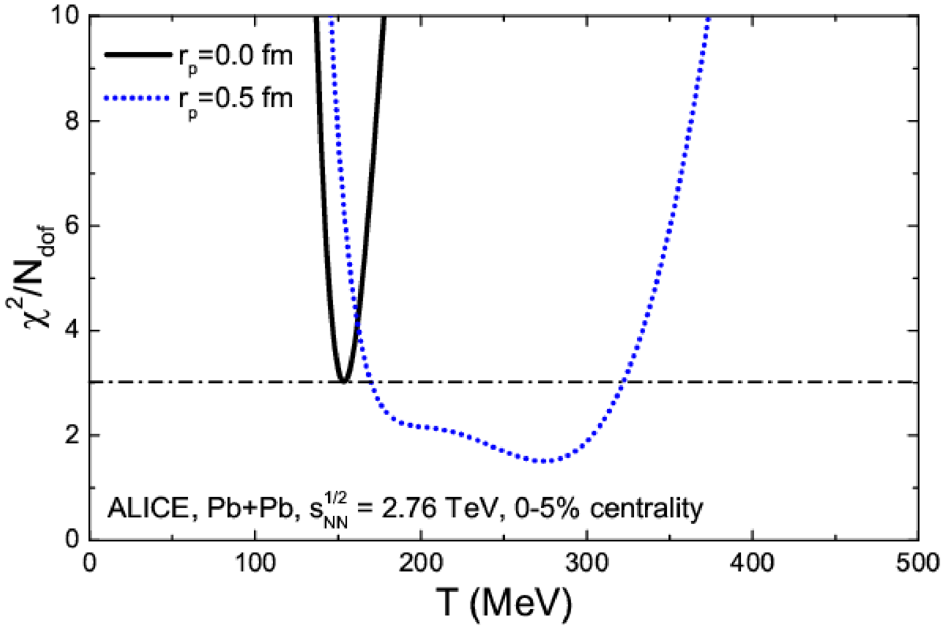
SHARE:

no EV effects

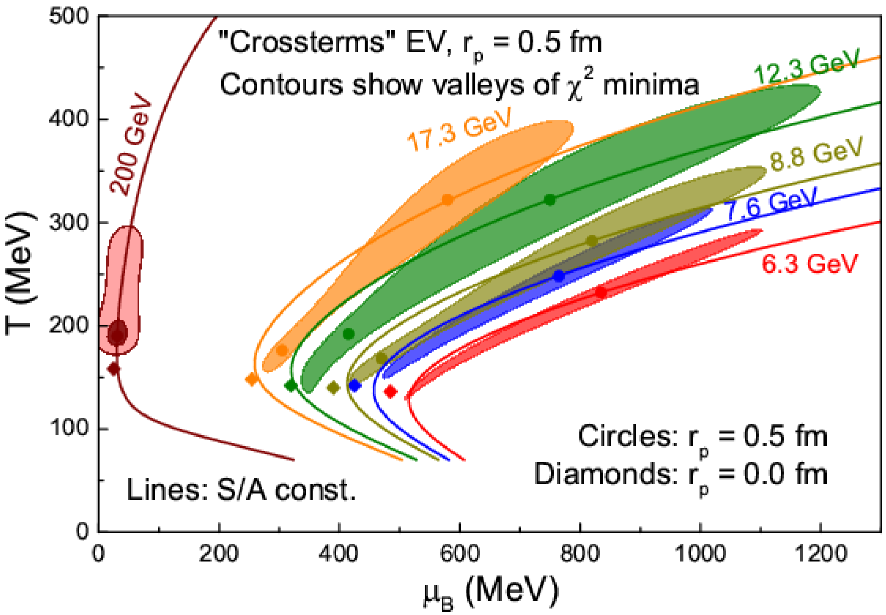
F. Bellini (ALICE collaboration), QM2018

Another extreme: bag model scaling

Bag model: $v_i \propto m_i$ [Chodos et al., PRD ’74; Kapusta et al., NPA ’83, PRC ’15]



[**V.V.**, H. Stoecker, 1512.08046]



[**V.V.**, H. Stoecker, 1606.06218]

Extraction of *T* and *μ* can be quite sensitive w.r.t EV corrections,

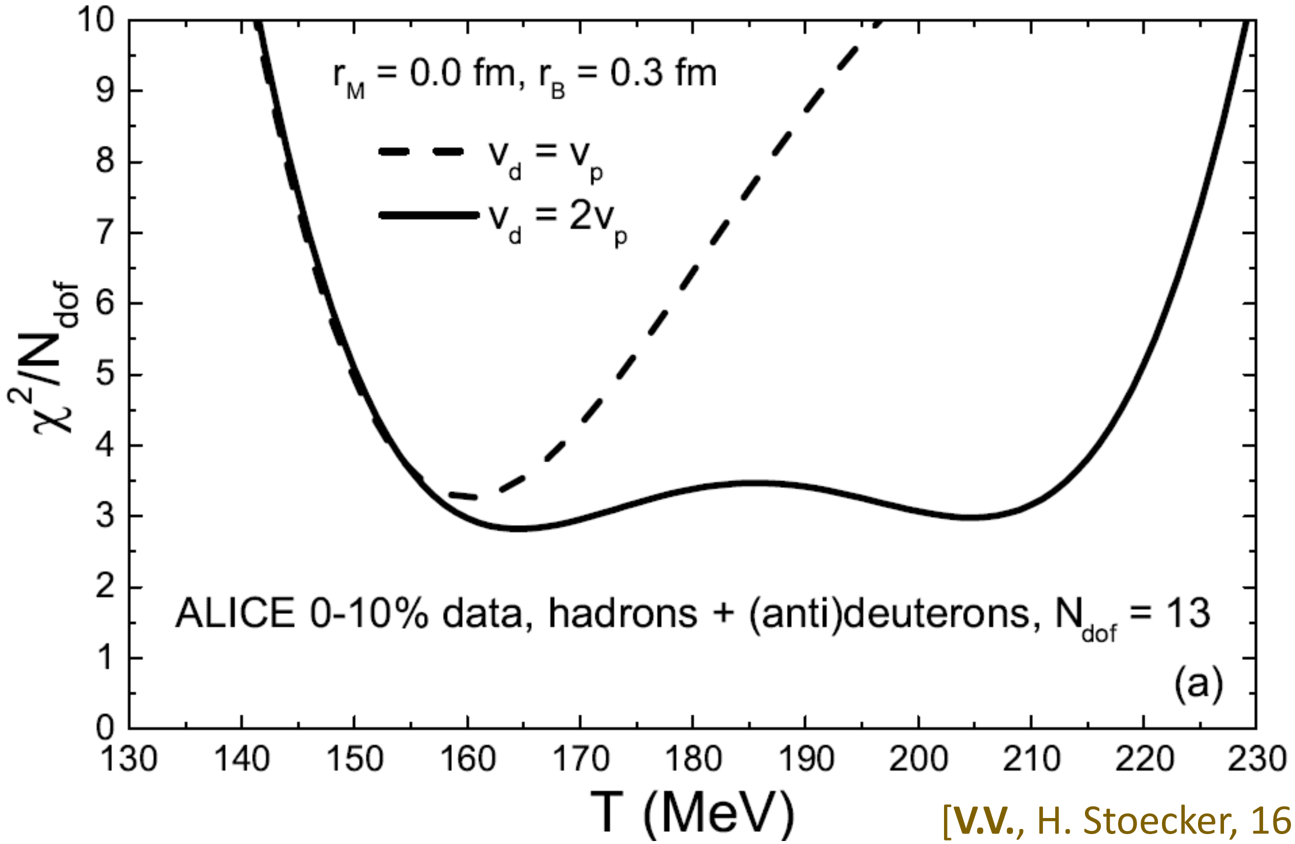
but entropy per baryon, S/A, is a robust observable

NB: This calculation disregards Hagedorn states needed to model the crossover transition **C. Greiner, talk Wednesday**

More moderate: two-component model

Two-component model: $r_M = 0$ fm, $r_B = 0.3$ fm [Andronic et al., 1201.0693]

Deuteron eigenvolume? Two options: $v_d = v_p$ and $v_d = 2v_p$



[**V.V.**, H. Stoecker, 1610.02346]

The 2nd minimum strikes again

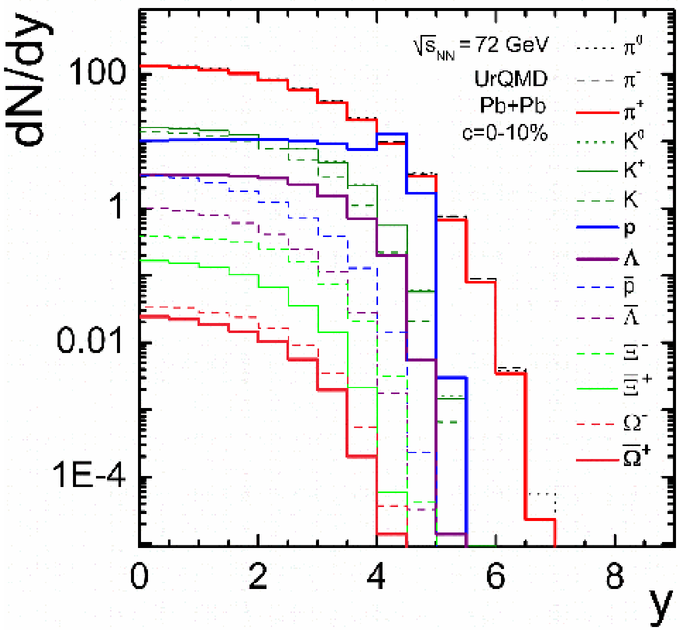
Rapidity scan

V. Begun, talk this afternoon

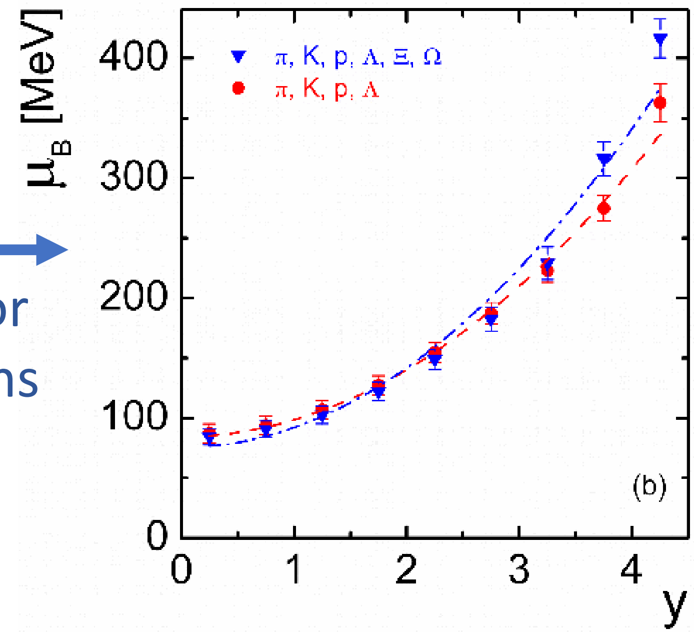
Fireballs at midrapidity: $\mu_B(y_s) \approx \mu_B(0) + b\, y_s^2$

RHIC @ $\sqrt{s_{NN}} = 200$ GeV: $\mu_B(y_s) \approx 25 + 11 y_s^2$ [MeV] [Becattini et al., 0709.2599]

Example: AFTER@LHC project: Pb+Pb collisions @ $\sqrt{s_{NN}} = 72$ GeV



Thermal fits for different dy bins



[Begun, Kikola, **V.V.**, Wielanek, 1806.01303]

Rapidity scan: complementary approach to scan QCD phase diagram

see also Li, Kapusta, 1604.08525; Brewer, Mukherjee, Rajagopal, Yin, 1804.10215

Summary

- New **Thermal-FIST** package provides most of the features used in thermal model analysis in a convenient way
- Broad resonances is a source of systematic uncertainty in HRG model, ‘proton anomaly’ is within this uncertainty
- Canonical statistical model captures multiplicity dependence of light nuclei and strange hadron production at LHC, ϕ/π and p/π ratios not captured
- Understanding effects of broad resonances and excluded volume interactions is important for precision studies

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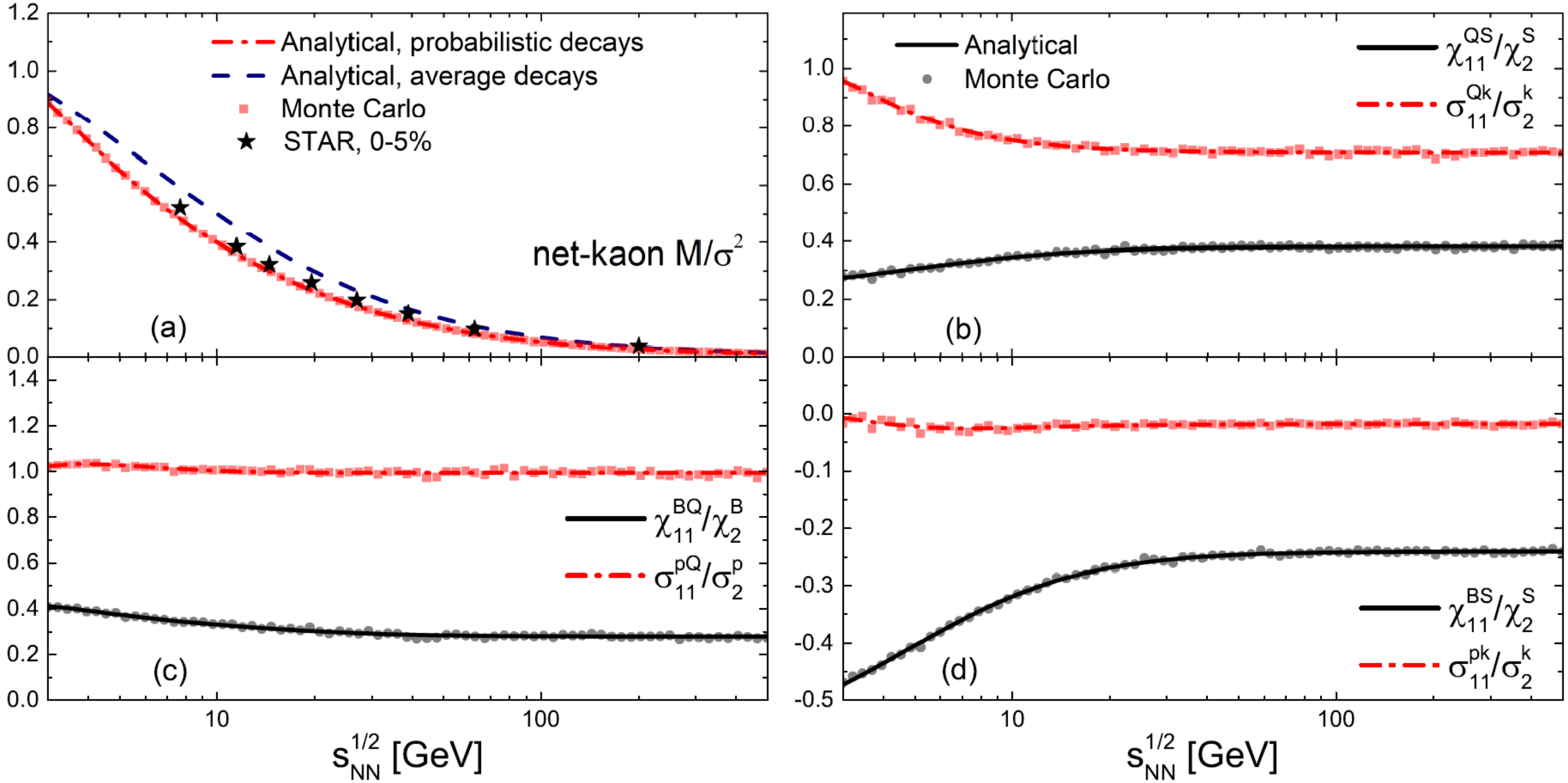
Thanks for your attention!

Backup slides

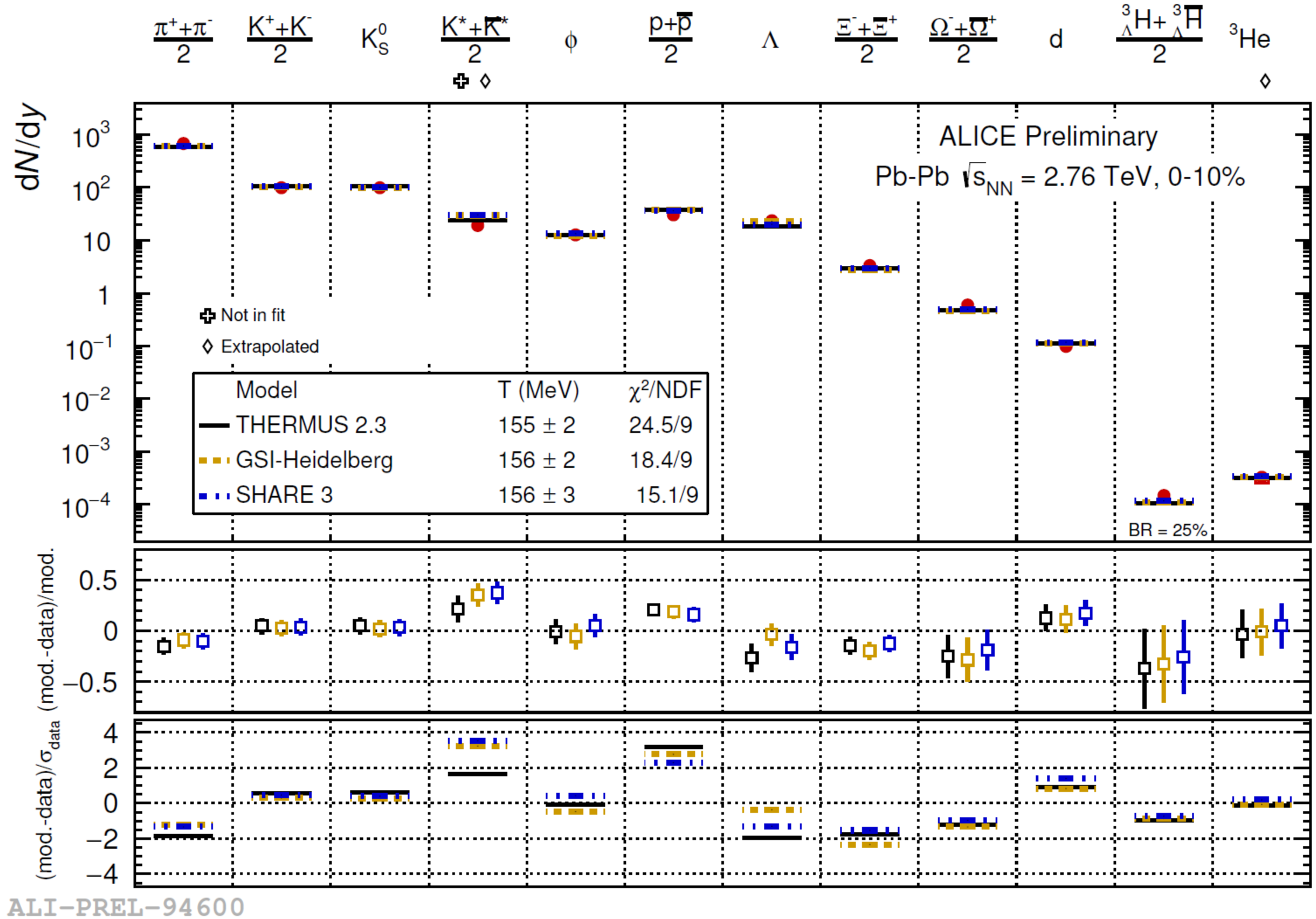
Particle number fluctuations and correlations

$$\langle \Delta N_i \, \Delta N_j \rangle_{c.e.} = \langle \Delta N_i^* \Delta N_j^* \rangle_{c.e.} + \sum_R \langle N_R \rangle \, \langle \Delta n_i \, \Delta n_j \rangle_R + \sum_R \langle \Delta N_i^* \, \Delta N_R \rangle_{c.e.} \, \langle n_j \rangle_R$$

$$+ \sum_R \langle \Delta N_j^* \, \Delta N_R \rangle_{c.e.} \, \langle n_i \rangle_R + \sum_{R,R'} \langle \Delta N_R \, \Delta N_{R'} \rangle_{c.e.} \, \langle n_i \rangle_R \, \langle n_j \rangle_{R'} \, .$$



Standard picture for Pb+Pb @ 2.76 TeV



ALICE collaboration (SQM 2015)

Similar results with *Thermal-FIST* and *Florence codes* [Becattini et al., 1605.09694]

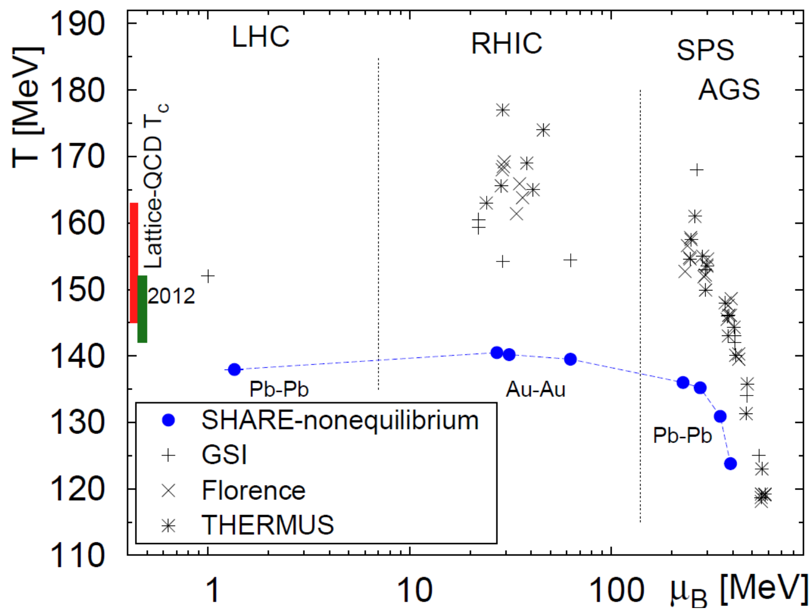
Consistent picture between codes for chem. equilibrium ideal HRG

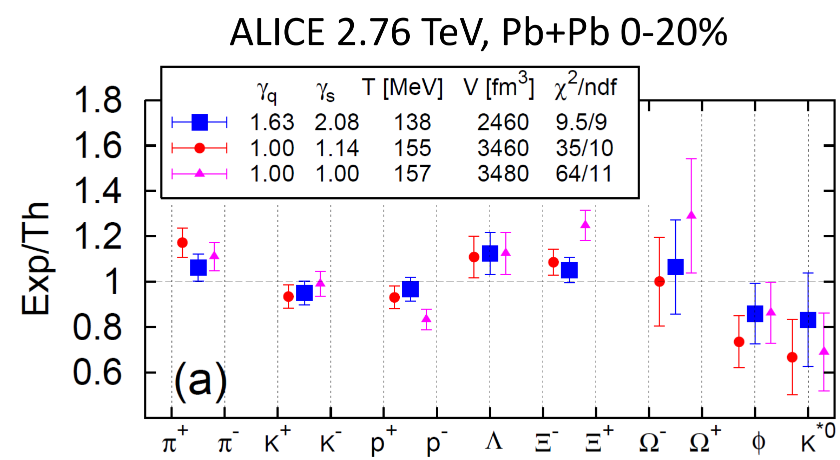
Alternative/extended scenarios

Chemical non-equilibrium model

In chemical non-equilibrium scenario $N_i^{\mathrm{hrg}} \propto (\gamma_q)^{|q_i|}(\gamma_s)^{|s_i|}$

E.g. hadronization of chem. non-eq. supercooled QGP [Letessier, Rafelski, '99]





[M. Petran et al., 1303.2098]

- smaller reduced χ^2 compared to chem. equilibrium scenario
- describes p_T-spectra of many hadrons [V. Begun et al., 1312.1487, 1405.7252]
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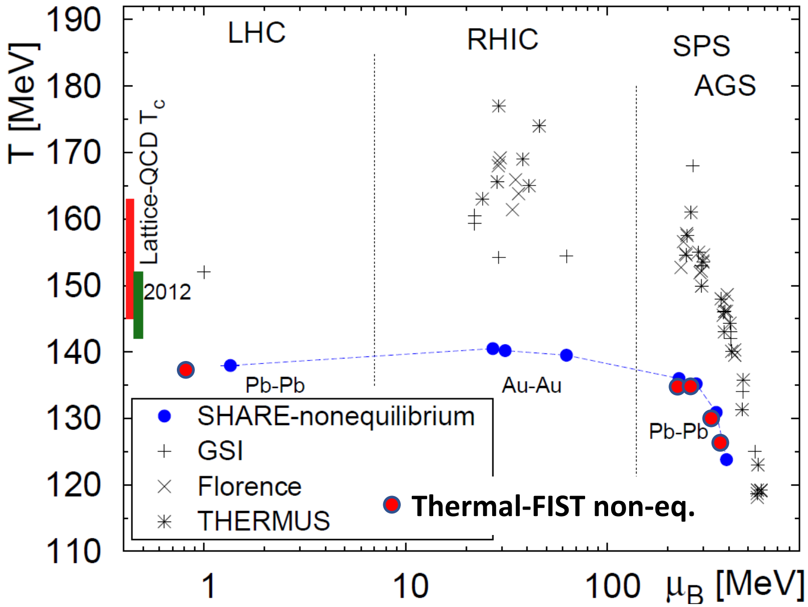

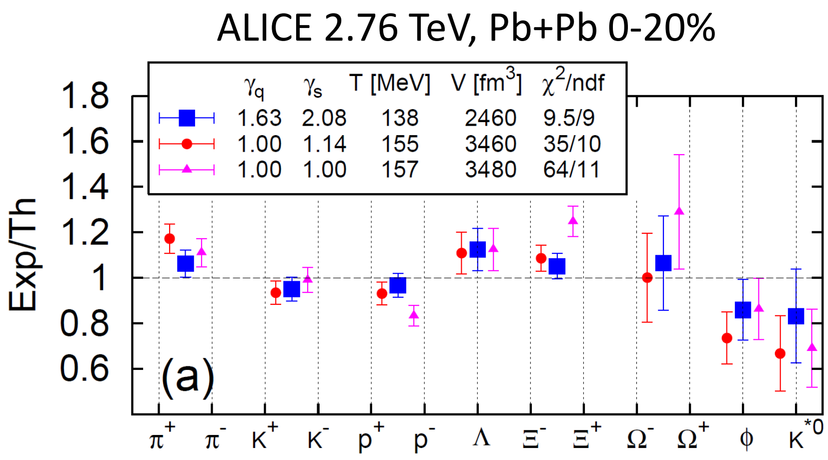

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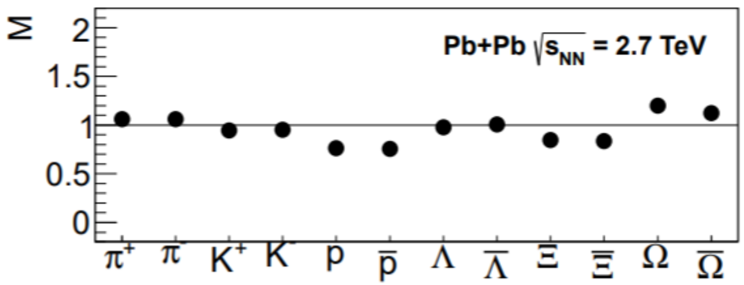
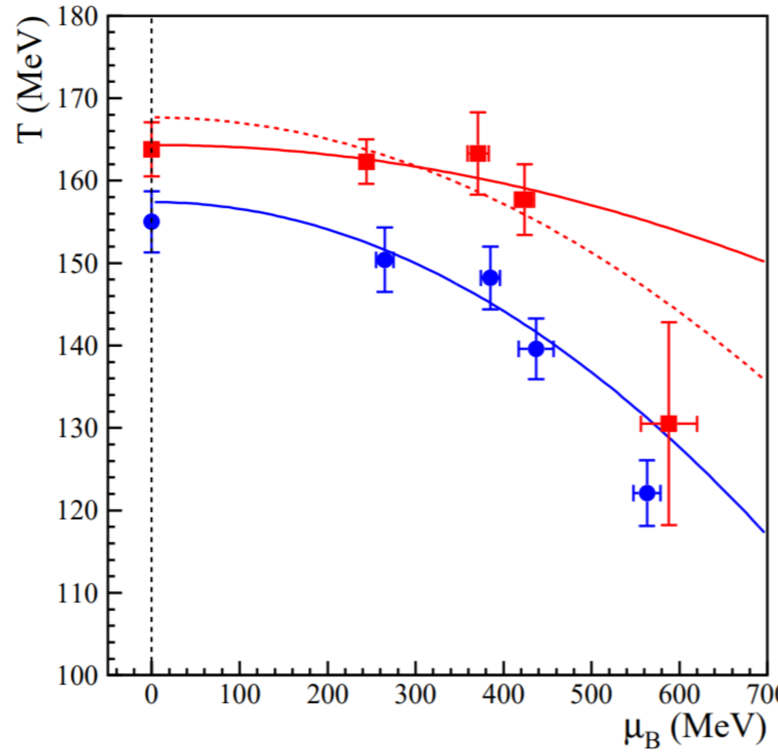
Influence of the hadronic phase

Modification of hadron yields in non-equilibrium hadronic phase

$B\bar{B}$ annihilation reduces (anti)proton yields [Steinheimer et al., 1203.5302]



	T(MeV)	μ_B(MeV)	γ_S	χ^2/NDF
Pb-Pb 20% central $\sqrt{s_{\rm NN}} = 2.7$ TeV				
Std. fit	156 ± 5	1 ± 12	1.09 ± 0.07	26.5/9
Mod. fit	166 ± 3	2 ± 6	0.98 ± 0.04	11.5/9
Pb-Pb 5% central $\sqrt{s_{\rm NN}} = 17.3$ GeV				
Std. fit	151 ± 4	266 ± 9	0.91 ± 0.05	26.9/11
Mod. fit	163 ± 4	250 ± 9	0.83 ± 0.04	20.4/11
Pb-Pb 5% central $\sqrt{s_{\rm NN}} = 8.7$ GeV				
Std. fit	148 ± 4	385 ± 11	0.78 ± 0.06	17.9/9
Mod. fit	161 ± 6	376 ± 15	0.72 ± 0.06	25.9/9
Pb-Pb 5% central $\sqrt{s_{\rm NN}} = 7.6$ GeV				
Std. fit	140 ± 1	437 ± 5	0.91 ± 0.01	22.4/7
Mod. fit	156 ± 5	426 ± 4	0.81 ± 0.00	14.7/7



[Becattini et al., 1212.2431, 1605.09694]

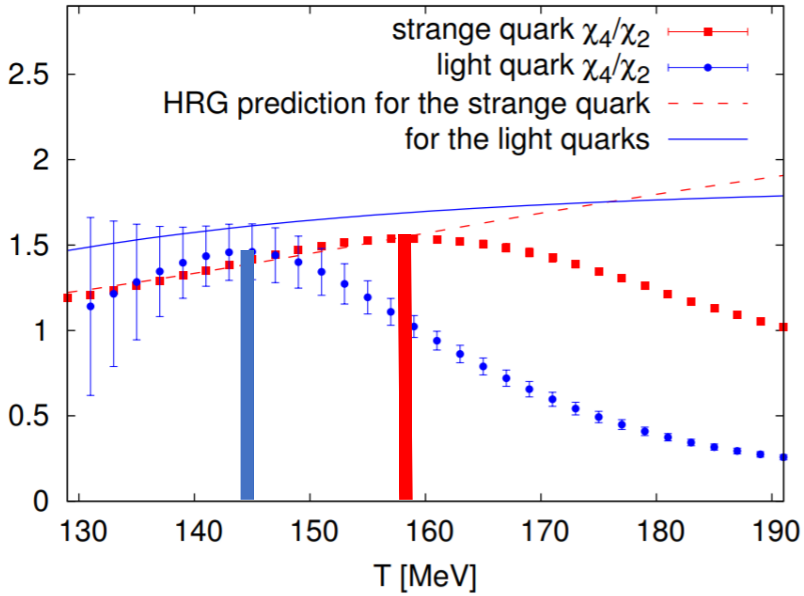
- somewhat better χ^2 and increase in T_{ch} by 10-15 MeV
- no backreaction, e.g. $5M \to B\bar{B}$, in UrQMD. What is its role?

Flavor hierarchy at freeze-out

QCD transition is a broad crossover

=> different "T_c" for different observables

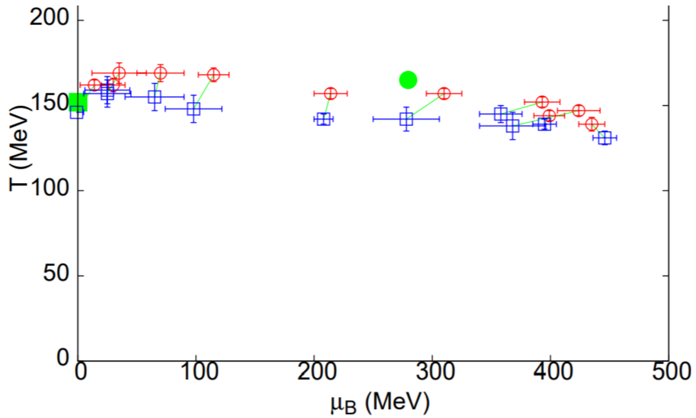
strange vs light number susceptibility

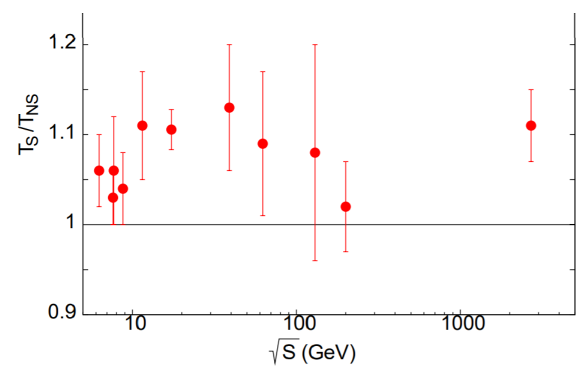


[R. Bellwied et al., 1305.6297]

2CFO scheme

[S. Chatterjee et al., 1306.2006]





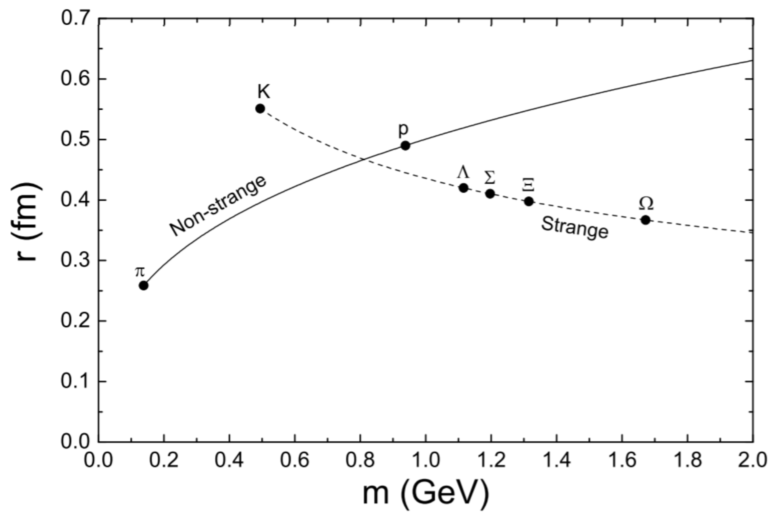
- higher T_f for strange particles than for non-strange
- effect may disappear if more strange baryons included

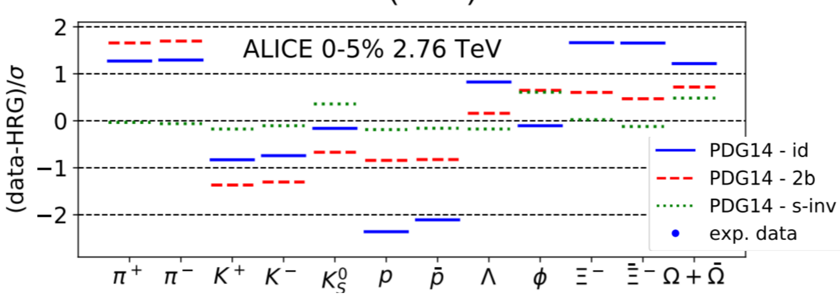
[Bazavov et al., 1404.6511, S. Chatterjee, 1708.08152]

Flavor hierarchy in hadron sizes

Alternative: Flavor hierarchy in hadron sizes [P. Alba et al., 1606.06542]

$v_i \propto m_i$ for non-strange, $v_i \propto m_i^{-1}$ for strange, excluded-volume HRG





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χ^2/N_{dof} = **0.88/7**

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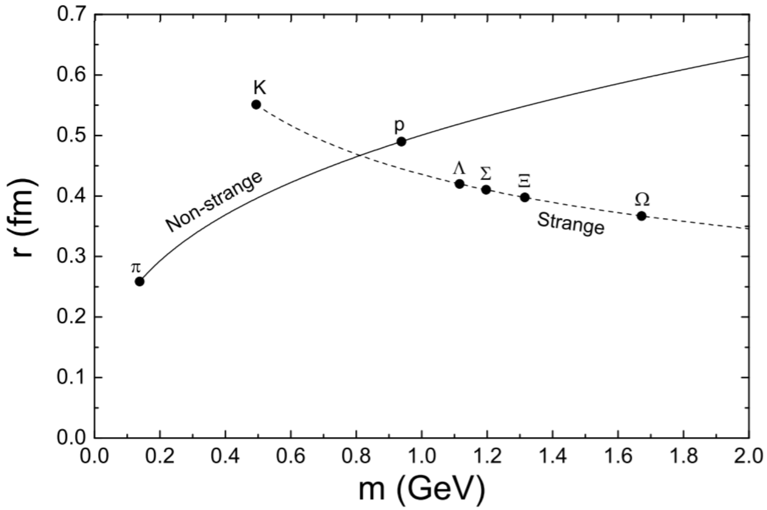

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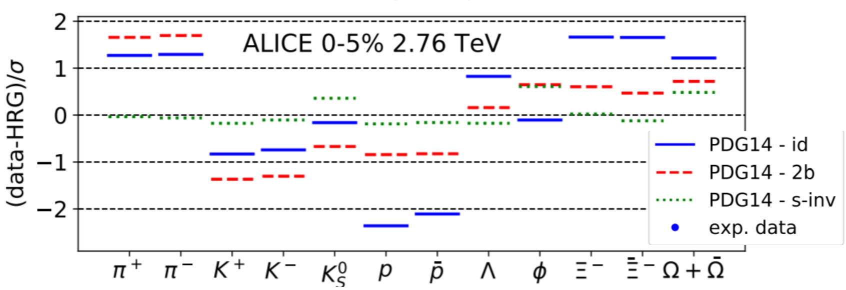

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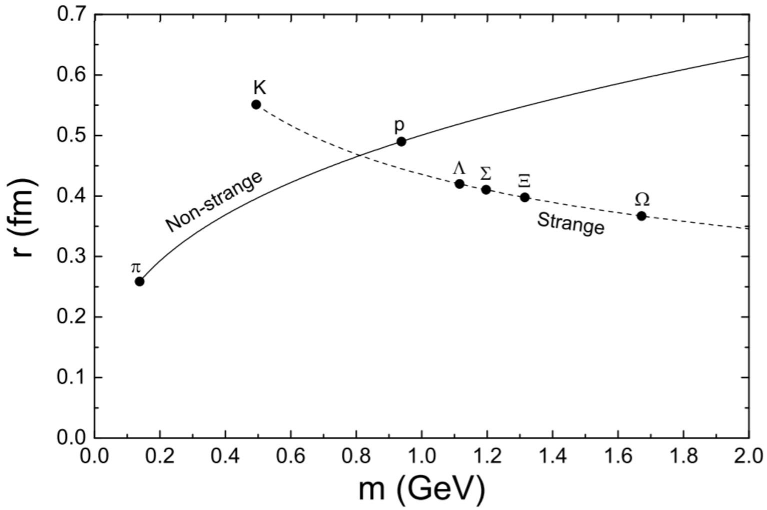

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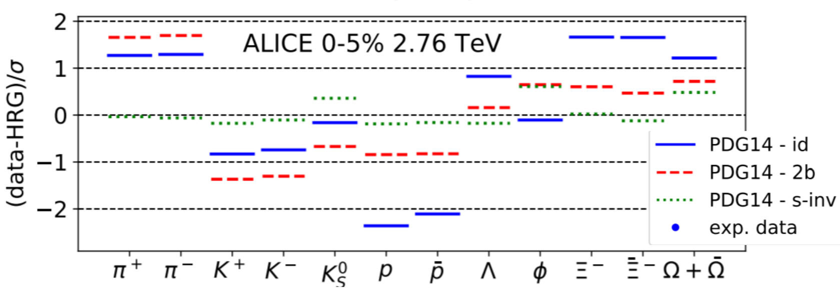

	$\chi^2/N_{\rm dof}$
STAR 200	$16.8/8 \simeq 2.1$
NA49 158	$70.1/10 \simeq 7.01$
NA49 80	$71.7/7 \simeq 10.2$
NA49 40	$44.2/8 \simeq 5.5$
NA49 30	$29.6/7 \simeq 4.2$

→

$\chi^2/N_{\rm dof}$
$6.5/8 \simeq 0.82$
$57.4/10 \simeq 5.7$
$28.3/7 \simeq 4.05$
$15.1/8 \simeq 1.8$
$7.08/7 \simeq 1.01$

- Significant improvement in fit quality across $\sqrt{s}$ and centralities
- Reflects systematics in data, exact physical reasons to be clarified

Hierarchy in baryon number?

Considering the ALICE 2.76 TeV Pb+Pb 0-10% data in ideal HRG model…

1) Fit of mesons + baryons + nuclei: $T_{ch} = 155 \pm 2$ MeV, χ^2/N_{dof} = 41.9/20

2) Fit of mesons + baryons: $T_{ch} = 155 \pm 2$ MeV, χ^2/N_{dof} = 36.7/12

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5) Fit of nuclei (d, ^{3}He, $^3_\Lambda$H, ^{4}He): $T_{ch} = \mathbf{161} \pm 4$ MeV, χ^2/N_{dof} = **2.4/6**

Similar results at other centralities

Rather different fit temperatures in different baryon number sectors…

More tension in the baryonic sector

Systematic uncertainties in the HRG model

Input hadron list and decay channels

- High-mass resonances and their decay channels poorly known
- Evidence for missing strange baryons for lattice QCD
  [A. Bazavov et al., 1404.6511; P. Alba et al., 1702.0113; S. Chatterjee, 1708.08152]

Modeling finite resonance widths

- Zero-width approx., energy (in)dependent Breit-Wigner, phase shifts

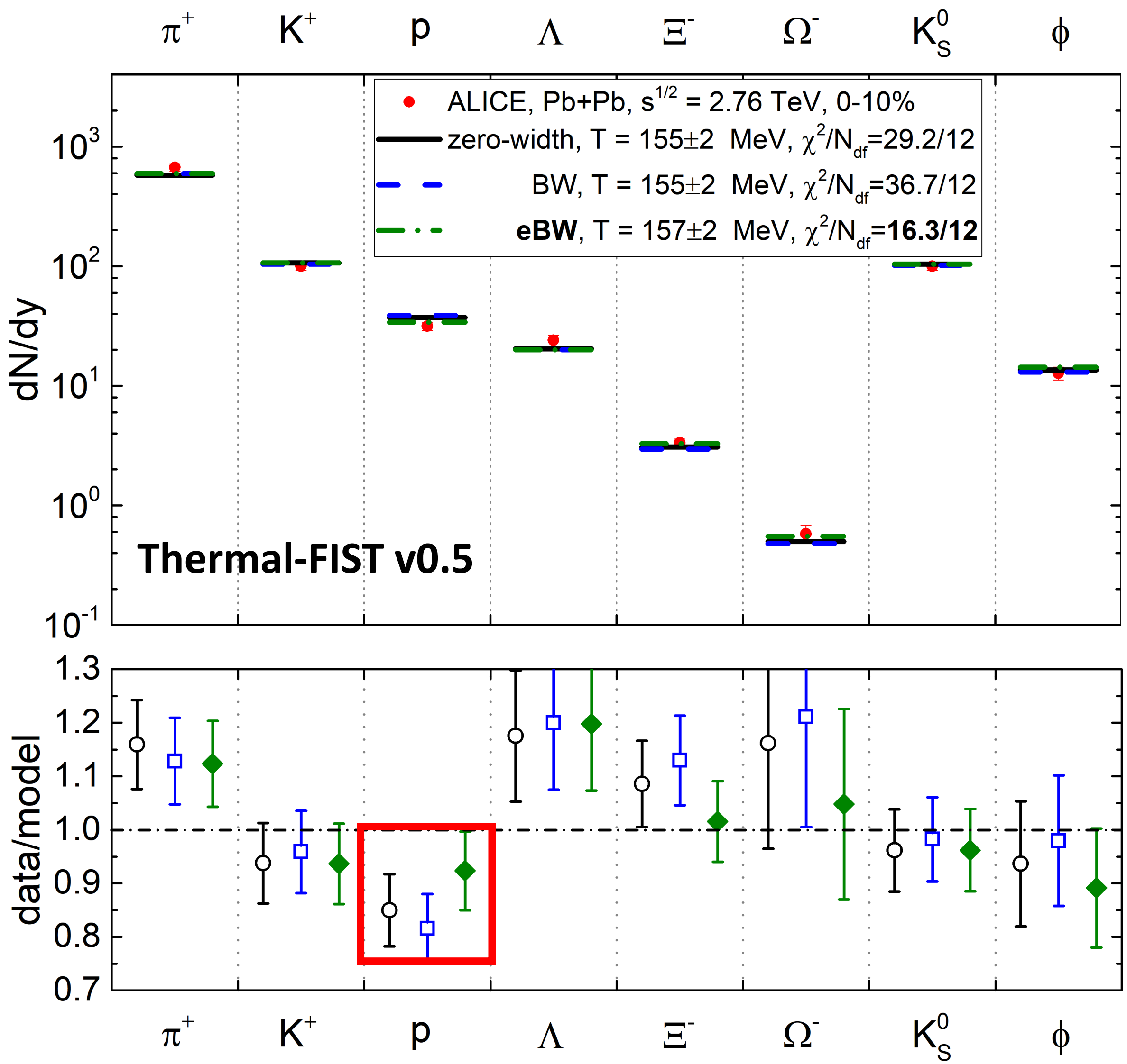
Excluded volume/van der Waals interaction effects

- Thermal fits affected when EV parameters differ between hadrons
  [**V.V.**, H. Stoecker, 1512.08046, 1606.06218]

In-medium hadron masses

- In-medium masses due to interactions/chiral symmetry restoration
  [D. Zschiesche et al., nucl-th/0209022; G. Aarts et al., 1703.09246]
- Needs reconciliation with vacuum masses actually measured

Modeling widths: effect on thermal fits



Significant improvement in the eBW scheme due to a reduced proton feeddown from Δ and N*

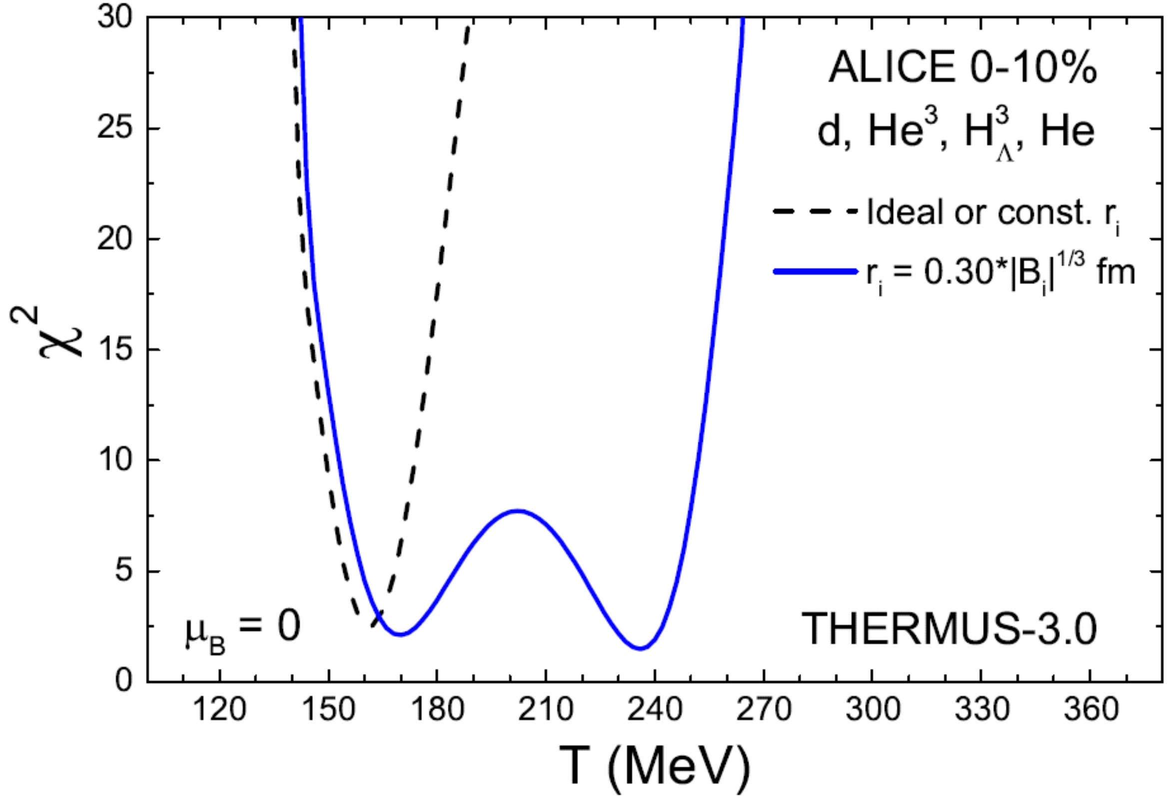
Modeling of wide resonances important!!

[**V.V.** et al., in preparation]

Fitting light nuclei only

One could forget about the hadrons and fit just the light nuclei

Advantage: No dependence on high-mass resonance spectrum and feeddown



Ideal HRG (or $v_i = \text{const.}$): $T_f = 160 \pm 5$ MeV

EV-HRG with $v_i = v|A_i|$: $T_f = 160 - 250$ MeV

Disadvantage: Fits are even more sensitive to EV corrections