

Statistical-thermal FIST package

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V.V., H. Stoecker, arXiv:1901.05249, Computer Physics Communications (accepted)

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

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Hadron resonance gas (HRG) at freeze-out

HRG: Equation of state of hadronic matter as a multi-component (non-)interacting gas of known hadrons and resonances

$$\ln Z \approx \sum_{i \in M,B} \ln Z_i^{id} = \sum_{i \in M,B} \frac{d_i V}{2\pi^2} \int_0^\infty \pm p^2 dp \ln \left[1 \pm \exp\left(\frac{\mu_i - E_i}{T}\right) \right]$$

Grand-canonical ensemble: $\mu_i = b_i \mu_B + q_i \mu_Q + s_i \mu_S$ **chemical equilibrium**



Thermal model:

Equilibrated hadron resonance gas at the chemical freeze-out stage of high-energy collisions

Model parameters:

T – temperature

 $\mu_{B_{J}} \mu_{Q_{J}} \mu_{S}$ – chemical potentials

V- system volume

© J. Cleymans

and many more aspects

Available thermal model codes:

- 1) **SHARE 3** [G. Torrieri, J. Rafelski, M. Petran, et al.] Since 2003 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.] Since 2004 C++/ROOT. Canonical ensemble, EV corrections, charm, nuclei open source: https://github.com/thermus-project/THERMUS

New development:



Thermal-FIST* (current version: v1.2.1) [V.V., H. Stoecker] *C++.* Chemical (non-)equilibrium, EV/vdW corrections, Monte Carlo, (higher-order) fluctuations, canonical ensemble, combinations of effects **open source:** https://github.com/vlvovch/Thermal-FIST *Since 2018* physics manual: arXiv:1901.05249

Using Thermal-FIST



The package is cross-platform (Linux, Mac, Windows, Android) Installation using **git** and **cmake**

```
# Clone the repository from GitHub
git clone https://github.com/vlvovch/Thermal-FIST.git
cd Thermal-FIST
# Create a build directory, configure the project with cmake
# and build with make
mkdir build
cd build
cmake ../
make
# Run the GUI frontend
./bin/QtThermalFIST
# Run the test calculations from the paper
./bin/examples/cpc1HRGTDep
./bin/examples/cpc2chi2
./bin/examples/cpc3chi2NEQ
./bin/examples/cpc4mcHRG
```

GUI requires free Qt5 framework, the rest of the package has no external dependencies Quick start guide Documentation Physics manual

Thermal-FIST



Graphical user interface for general-purpose thermal model applications



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

"Thanks for reproducing my results!"

F. Becattini

FIST in THERMUS mode: cross-check







FIST in THERMUS mode: cross-check





FIST: Fist IS Thermus



FIST in THERMUS mode: cross-check





FIST: Fist IS Thermus

and more

FIST and Jupyter notebooks



Usual usage: through GUI or compiled C++ macros

NEW: Interactive notebooks through Jupyter (xeus kernel and ROOT-cling)*



*Since version 1.2.1, example at github.com/vlvovch/FIST-jupyter

Thermal model aspects in **FIST**



- Extensions of the HRG model
 - finite resonance widths
 - repulsive interactions (excluded volume)
 - van der Waals interactions (*criticality*)
 - particle number fluctuations and correlations
 - chemical non-equilibrium (γ_q, γ_s) a la Rafelski
- Equation of state
- Canonical statistical model (CSM)
 - (local) (selective) exact conservation of conserved charges
 - uniform description of hadrochemistry from small to large systems
- Monte Carlo generator (Blast-wave, canonical ensemble,...)
- Hadronic phase and dynamical freeze-out
 - Partial chemical equilibrium
 - Suppression of resonance yields
 - Evolution of light nuclei abundances via the Saha equation



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Finite resonance widths



$$n_{i}(T, \mu; m_{i}) \rightarrow \int_{m_{i}^{max}}^{m_{i}^{max}} dm \,\rho_{i}(m) \,n_{i}(T, \mu; m)$$
1) Zero-width approximation
Simplest and common possibility
2) Energy-(in)dependent Breit-Wigner
$$\rho_{i}^{BW}(m) = A_{i} \frac{2 m m_{i} \Gamma_{i}}{(m^{2} - m_{i}^{2})^{2} + m_{i}^{2} \Gamma_{i}^{2}}}{\Gamma_{i \rightarrow j}(m) = b_{i \rightarrow j} \Gamma_{i} \left[1 - \left(\frac{m_{i \rightarrow j}^{thr}}{m}\right)^{2}\right]^{L_{i \rightarrow j}+1/2}}$$

suppression of the spectral strength at the threshold

Alternative: S-matrix approach using phase shifts $\rho_i(m) \propto \frac{\partial \delta(m)}{\partial m}$ Usually based on measured scattering phase shifts

[cf. Huovinen et al., PLB '17; P.M. Lo et al, PLB '19]

Finite resonance widths: data description





Energy-dependent Breit-Wigner leads to a 15% suppression of proton yields also affected: 10% decrease of Λ

This is enough to describe the 'proton yield anomaly' at 2.76 TeV*

*but beware of the 5 TeV data, see below

⁴He

V.V., Gorenstein, Stoecker, 1807.02079 source code at github.com/vlvovch/1807.02079

Multiplicity dependence of hadrochemistry





- Hadron yield ratios exhibit multiplicity dependence
- Grand-canonical picture predicts no multiplicity dependence
- Ratios appear to approach a plateau at high-multiplicities
 → grand-canonical plateau?
- Can multiplicity-dependence be considered in a macroscopic canonical statistical model?

Canonical statistical model (CSM)



Exact conservation of *B*, *Q*, *S* in a correlation volume *V*_C [Rafelski, Danos, et al., PLB '80; Hagedorn, Redlich, ZPC '85] $\mathcal{Z}(B,Q,S) = \int_{-\pi}^{\pi} \frac{d\phi_B}{2\pi} \int_{-\pi}^{\pi} \frac{d\phi_Q}{2\pi} \int_{-\pi}^{\pi} \frac{d\phi_S}{2\pi} e^{-i(B\phi_B + Q\phi_Q + S\phi_S)} \exp\left[\sum_j z_j^1 e^{i(B_j\phi_B + Q_j\phi_Q + S_j\phi_S)}\right]$ $z_j^1 = V_c \int dm \rho_j(m) d_j \frac{m^2 T}{2\pi^2} K_2(m/T) \qquad \langle N_j^{\text{prim}} \rangle^{\text{ce}} = \frac{Z(B - B_j, Q - Q_j, S - S_j)}{Z(B, Q, S)} \langle N_j^{\text{prim}} \rangle^{\text{gce}}$

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

Implemented in Thermal-FIST for a full HRG

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Exact conservation around midrapidity, $V_C = k dV/dy$. How large is k?

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Net-proton fluctuations affected by baryon number conservation [Braun-Munzinger, Rustamov, Stachel, 1612.00702]

$$rac{\kappa_2(\mathsf{p}-\overline{\mathsf{p}})}{\langle\mathsf{p}
angle+\langle\overline{\mathsf{p}}
angle}\simeq 1-rac{\langle\mathsf{p}
angle}{k\,dN_B/dy}$$

Using ALICE preliminary data for net-p fluctuations [Rustamov, 1704.05329] one obtains $k \sim 3-4$ for most centrality bins in Pb-Pb collisions [V.V., Dönigus, Stoecker, 1906.03145] 12

"Vanilla" CSM at LHC



 $T_{ch} = 155$ MeV, $V_C = 3dV/dy$, multiplicity dependence driven by V_C only



Fair for hyperons, protons and kaons worse, ϕ goes in the opposite direction

[**V.V.**, Dönigus, Stoecker, 1906.03145]

Full CSM analysis



 γ_S CSM: $V_C = 3dV/dy$, fit T_{ch} and γ_S at each centrality in p-p, p-Pb, Pb-Pb



Canonical suppression and strangeness saturation important below $dN_{ch}/d\eta \approx 100$

Full CSM analysis: yields





Relative accuracy of $\gamma_s CSM$ is ~15% across all multiplicity bins

[V.V., Dönigus, Stoecker, 1906.03145]

Hadronic phase





- At $T_{ch} \approx 150 160$ MeV inelastic collisions cease, yields of hadrons frozen
- Kinetic equilibrium maintained down to $T_{kin} \approx 100 120$ MeV through (pseudo-)elastic scatterings

[e.g., E. Shuryak, Rev. Mod. Phys. 89, 035001 (2017)]



Expansion of hadron resonance gas in partial chemical equilibrium at $T < T_{ch}$ [H. Bebie, P. Gerber, J.L. Goity, H. Leutwyler, Nucl. Phys. B '92; C.M. Hung, E. Shuryak, PRC '98]

Chemical composition of stable hadrons is fixed, kinetic equilibrium maintained through pseudo-elastic resonance reactions $\pi\pi \leftrightarrow \rho$, $\pi K \leftrightarrow K^*, \pi N \leftrightarrow \Delta$, etc.

Effective chemical potentials:

 $\tilde{\mu}_j = \sum_{i \in \text{stable}} \langle n_i \rangle_j \mu_i, \quad \langle n_i \rangle_j - \text{mean number of hadron } i \text{ from decays of hadron } j, \quad j \in \text{HRG}$

Conservation laws:



 $\label{eq:linear} Numerical implementation is in Thermal-FIST development branch $$ https://github.com/vlvovch/Thermal-FIST/tree/pce $$ the second second$

Partial chemical equilibrium at the LHC





[V.V., K. Gallmeister, J. Schaffner-Bielich, C. Greiner, 1903.10024]

"Initial conditions" from thermal fits with Thermal-FIST to 0-10% ALICE hadron yields $T_{ch} = 155$ MeV, $V_{ch} = 4700$ fm³

Light nuclei in the hadronic phase



Detailed balance for nuclear reactions, $X + A \leftrightarrow X + \sum_i A_i$, X is e.g. a pion $\frac{n_A}{\prod_i n_{A_i}} = \frac{n_A^{\text{eq}}}{\prod_i n_{A_i}^{\text{eq}}}, \quad \Leftrightarrow \quad \mu_A = \sum_i \mu_{A_i}, \quad \text{e.g. } \mu_d = \mu_p + \mu_n, \quad \mu_{3\text{He}} = 2\mu_p + \mu_n, \quad \dots$ [V.V., K. Gallmeister, J. Schaffner-Bielich, C. Greiner, 1903.10024] Saha equation 10⁻² d/p 10⁻³ NE/p Yield ratios 10⁻⁴ ³He/p ΞΞ/p $N\Omega/p$ 10⁻⁵ ³_^H/p 10⁻⁶ 10⁻⁷) (a) ⁴He/p (b) ⁴_AH/p, ⁴_AHe/p 10⁻⁸ T_{kiņ} 10⁻⁹ 130 80 90 100 110 120 140 150 80 90 100 110 120 130 140 150 70 T [MeV] T [MeV]

Deviations from thermal model predictions are moderate despite significant cooling and dilution. Is this the reason for why thermal model works so well?

Resonance suppression in hadronic phase

Yields of resonances are *not* conserved in partial chemical equilibrium E.g. K^{*} yield dilutes during the cooling through reactions $\pi K \leftrightarrow K^*$



At $T \approx T_{kin}$ the suppressed resonance yields agree quite well with ALICE/RHIS/SPS data for central A+A collisions

This implies significant resonance regeneration in the hadronic phase

5 TeV Pb-Pb data





5 TeV Pb-Pb data





FIST v1.2 (zero-width): $T_{ch} = 151 \pm 2$ MeV, $\chi^2/NDF = 47.4/9$ **FIST v1.2** (eBW): $T_{ch} = 152 \pm 2$ MeV, $\chi^2/NDF = 41.9/9$

A

Flavor hierarchy at freeze-out

QCD transition is a broad crossover => different " T_c " for different observables?



STO N

Flavor hierarchy at freeze-out

QCD transition is a broad crossover => different " T_c " for different observables?



Flavor hierarchy implementation in FIST:

- At $T = T_S$ inelastic strangeness reactions freeze, yields of strange hadrons frozen
- At $T_{NS} < T_S$ yields of all light-flavored stable hadrons freeze out
- From T_S to T_{NS} evolution in partial chemical equilibrium of strangeness, strange hadrons, and resonances decaying into them, attain fugacity factors









Three global fit parameters: T_S , V_S , and T_{NS}





Three global fit parameters: T_S , V_S , and T_{NS}



Precision data paves the way to test new scenarios

*no light nuclei here



- **Thermal-FIST** is a user-friendly open source package for general purpose thermal model applications with a modular structure.
- Usage:
 - Graphical user interface
 - C++ scripts
 - Jupyter notebooks

• Highlights of FIST results for ALICE

- Resonance widths as a possible solution to 'proton yield anomaly'
- Canonical statistical model description of p-p, p-Pb, and Pb-Pb collisions
- Formation of light nuclei deep in the hadronic phase via the Saha equation
- Suppression of resonance yields as a consequence of partial chemical equilibrium
- A unified description of the flavor hierarchy in the chemical freeze-out



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Thanks for your attention!

Backup slides

Two experimental observations at the LHC

1. Measured yields are described by thermal model at $T_{ch} \approx 155 \text{ MeV}^*$



2. Spectra described by blast-wave model at $T_{kin} \approx 100 - 120 \text{ MeV}^*$



[ALICE collaboration, PRC 93, 024917 (2016)]

What happens between T_{ch} and T_{kin} ?

Big Bang vs "Little Bangs"



- Hadrons (nucleons) form and "freeze-out" chemically before nuclei
- Bosons (photons or pions) catalyse nucleosynthesis

e.g. $p + n \leftrightarrow d + \gamma$ vs $p + n + \pi \leftrightarrow d + \pi$

LHC nucleosynthesis: simplified setup

- Chemical equilibrium lost at $T_{ch} = 155$ MeV, abundances of nucleons are frozen and acquire effective fugacity factors: $n_i = n_i^{eq} e^{\mu_N/T}$
- Isentropic expansion driven by effectively massless mesonic d.o.f.

$$rac{V}{V_{\mathsf{ch}}} = \left(rac{T_{\mathsf{ch}}}{T}
ight)^3$$
, $\mu_N \simeq rac{3}{2} \ T \ \mathsf{ln} \left(rac{T}{T_{\mathsf{ch}}}
ight) + m_N \ \left(1 - rac{T}{T_{\mathsf{ch}}}
ight)$

• Detailed balance for nuclear reactions, $X + A \leftrightarrow X + \sum_i A_i$, X is e.g. a pion

$$\frac{n_{A}}{\prod_{i} n_{A_{i}}} = \frac{n_{A}^{eq}}{\prod_{i} n_{A_{i}}^{eq}}, \quad \Leftrightarrow \quad \mu_{A} = \sum_{i} \mu_{A_{i}}, \quad \text{e.g.} \quad \mu_{d} = \mu_{p} + \mu_{n}, \quad \mu_{3}_{He} = 2\mu_{p} + \mu_{n}, \quad \dots$$

Saha equation
$$X_{A} = d_{A} \left[(d_{M})^{A-1} \zeta(3)^{A-1} \pi^{\frac{1-A}{2}} 2^{-\frac{3+A}{2}} \right] A^{5/2} \left(\frac{T}{m_{N}} \right)^{\frac{3}{2}(A-1)} \eta_{B}^{A-1} \exp\left(\frac{B_{A}}{T} \right)$$
$$d_{M} \sim 11 - 13, \quad \eta_{B} \simeq 0.03$$

BBN:
$$X_A = d_A \left[\zeta(3)^{A-1} \pi^{\frac{1-A}{2}} 2^{\frac{3A-5}{2}} \right] A^{\frac{5}{2}} \left(\frac{T}{m_N} \right)^{\frac{1}{2}(A-1)} \eta^{A-1} X_p^Z X_n^{A-Z} \exp\left(\frac{B_A}{T} \right)$$

[E. Kolb, M. Turner, "The Early Universe" (1990)] 8

(Simplified) Saha equation vs thermal model

Saha equation:

Thermal model:

Strong exponential dependence on the temperature is eliminated in the Saha equation approach

Further, quantitative applications require numerical treatment of full spectrum of *massive* mesonic and baryonic resonances

LHC deuteron-synthesis

PHYSICAL REVIEW C 99, 044907 (2019)

Editors' Suggestion

Featured in Physics

Microscopic study of deuteron production in PbPb collisions at $\sqrt{s} = 2.76$ TeV via hydrodynamics and a hadronic afterburner

Dmytro Oliinychenko,¹ Long-Gang Pang,^{1,2} Hannah Elfner,^{3,4,5} and Volker Koch¹ ¹Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, California 94720, USA ²Physics Department, University of California, Berkeley, California 94720, USA ³Frankfurt Institute for Advanced Studies, Ruth-Moufang-Strasse 1, 60438 Frankfurt am Main, Germany ⁴Institute for Theoretical Physics, Goethe University, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany ⁵GSI Helmholtzzentrum für Schwerionenforschung, Planckstr. 1, 64291 Darmstadt, Germany



FIG. 1. Deuteron-pion interaction cross sections from SAID database [40] and partial wave analysis [41] are compared to our parametrizations (Tables II and III in the Appendix). Inelastic $d\pi \leftrightarrow$



FIG. 5. Reaction rates of the most important $\pi d \leftrightarrow \pi pn$ reaction in forward and reverse direction.

Law of mass action at work

Modeling widths: Effect on hadron yields





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, $V_{c} \neq dV/dy$ Causality argument: exact conservation across a few units of rapidity?

New application: CSM for **light nuclei**

- Suppression of nuclei-toproton ratios at low multiplicities
- For these observables sufficient to enforce exact baryon conservation only



CSM at LHC: light nuclei





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

Excluded volume corrections



Notion that hadrons have finite eigenvolume suggested a while ago [R. Hagedorn, J. Rafelski, PLB '80]

Excluded volume model: $V \rightarrow V - bN \Rightarrow$ 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



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

Another extreme: bag model scaling





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



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

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

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



Rapidity scan: complementary approach to scan QCD phase diagram see also Li, Kapusta, 1604.08525; Brewer, Mukherjee, Rajagopal, Yin, 1804.10215