

# THERMUS\* – A Thermal Model Package for ROOT

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THERMUS, a package of C++ classes and functions allowing thermal model analyses to be performed within the object-oriented ROOT framework of analysis, is introduced.

## I. INTRODUCTION

With the appropriate choice of ensemble, the statistical-thermal model has proved extremely successful in describing the hadron multiplicities and momentum spectra observed in relativistic collisions of both heavy ions and elementary particles over a wide range of energies [1, 2, 3, 4, 5, 6, 7, 8, 9, 10].

This success motivated the development of THERMUS– a thermal model analysis package of C++ classes and functions for incorporation into the object-oriented ROOT framework [11]. Since all THERMUS classes inherit from the ROOT base class `TObject`, they can be fully integrated into the interactive ROOT environment. In this way, one has access to all of the ROOT functionality in a thermal analysis.

At present three distinct thermal model formalisms are implemented in THERMUS: the grand-canonical ensemble, in which baryon number ( $B$ ), strangeness ( $S$ ) and charge ( $Q$ ) are conserved on average; a strangeness-canonical ensemble, in which strangeness is exactly conserved while  $B$  and  $Q$  are treated grand-canonically; and, finally, a fully canonical ensemble in which  $B$ ,  $S$  and  $Q$  are each exactly conserved. The structure of THERMUS is such that extensions to include the quantum numbers carried by the heavier quarks will be easily achieved.

In this paper we begin with an overview of the thermal model, as applicable to THERMUS, before describing in some detail the structure of the package.

## II. OVERVIEW OF THE STATISTICAL-THERMAL MODEL

The statistical-thermal model assumes that at freeze-out all hadrons in the hadron gas resulting from a high energy collision follow equilibrium distributions. The conditions at chemical freeze-out (when inelastic collisions cease) are given by the hadron abundances, while the particle spectra offer insight into the conditions at thermal freeze-out (when elastic collisions cease). Since THERMUS currently performs only chemical analyses, we will defer discussion of momentum spectra analysis until THERMUS has been extended to include such functionality.

### A. The Statistical Formalisms

Once evaluated, the hadron gas partition function gives all primordial thermodynamic quantities of the system by simple differentiation. The exact form of the partition function, however, depends on the statistical ensemble under consideration.

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\* <http://hep.phy.uct.ac.za/THERMUS/>

### 1. The Grand-canonical Ensemble

This ensemble is the most widely used in applications to heavy ion collisions [1, 2, 3, 4, 5, 6, 7, 8]. Within the grand-canonical ensemble, the quantum numbers of the system are conserved on average through the action of chemical potentials. In other words, the baryon content,  $B$ , strangeness content,  $S$  and charge content,  $Q$ , are fixed on average by  $\mu_B$ ,  $\mu_S$  and  $\mu_Q$  respectively. For each of these chemical potentials one can write a corresponding fugacity using the standard prescription  $\lambda = e^{\mu/T}$ , where  $T$  is the temperature of the system.

As an example, the density of hadron species  $i$  with quantum numbers  $B_i$ ,  $S_i$  and  $Q_i$ , spin-isospin degeneracy factor,  $g_i$ , and mass,  $m_i$ , emitted directly from a fireball at temperature  $T$  is,

$$n_i(T, \mu_B, \mu_S, \mu_Q, \gamma_S) = g_i \int \frac{d^3p}{(2\pi)^3} \left[ \gamma_S^{-|\tilde{S}_i|} e^{\sqrt{m_i^2 + p^2}/T} \lambda_B^{-B_i} \lambda_S^{-S_i} \lambda_Q^{-Q_i} \pm 1 \right]^{-1}, \quad (2.1)$$

where, in addition to the fugacities already introduced, we include  $\gamma_S$ , raised to the power  $-|\tilde{S}_i|$  (with  $|\tilde{S}_i|$  the number of strange and anti-strange quarks in hadron species  $i$ ), to allow for possible incomplete equilibration in the strange sector [12]. In Equation 2.1 quantum statistics is taken into account; the positive sign refers to fermions, while the negative sign is applicable to bosons. In the Boltzmann approximation, the density can be analytically evaluated as a second order modified Bessel function of the second kind,

$$\tilde{n}_i(T, \mu_B, \mu_S, \mu_Q, \gamma_S) = \frac{g_i}{2\pi^2} m_i^2 T \lambda_B^{B_i} \lambda_S^{S_i} \lambda_Q^{Q_i} \gamma_S^{|\tilde{S}_i|} K_2 \left( \frac{m_i}{T} \right). \quad (2.2)$$

The quantum-statistical result requires either an infinite summation over such  $K_2$ -functions or else a numerical integration.

The chemical potentials  $\mu_S$  and  $\mu_Q$  are typically constrained in applications of the model by the initial strangeness and baryon-to-charge ratio in the system under consideration.

### 2. The Strangeness-canonical Ensemble

As the number of particles in the fireball drops, so the conservation of quantum numbers on average becomes less acceptable. Since strangeness is typically the least abundant of the quantum numbers under consideration, the exact treatment of the  $S$  quantum number has first to be imposed. This is enforced in the strangeness-canonical ensemble. In the expression for the strangeness-canonical partition function,  $Z_S$ , only those states within the volume,  $V$ , with exactly the desired strangeness content,  $S$ , are allowed.

The primordial particle density of hadron species  $i$ ,  $n_i^S$ , is then, assuming Boltzmann statistics, proportional to the associated grand-canonical density of the hadron  $\tilde{n}_i$  [13, 14],

$$n_i^S(T, \mu_B, S, \mu_Q, \gamma_S, V) = \left( \frac{Z_{S-S_i}}{Z_S} \right) \tilde{n}_i(T, \mu_B, \mu_S = 0, \mu_Q, \gamma_S), \quad (2.3)$$

with the partition function expressed in terms of modified Bessel functions of the first kind as

$$Z_S = Z_0 \times \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} I_{|3m+2n-S|}(x_1) I_{|n|}(x_2) I_{|m|}(x_3) y_1^{-(3m+2n-S)} y_2^n y_3^m, \quad (2.4)$$

where  $Z_0$  is the contribution of the non-strange hadrons and

$$x_q = 2 \cdot \sqrt{k_{+q} k_{-q}} \quad \text{and} \quad y_q = \sqrt{\frac{k_{+q}}{k_{-q}}} \quad (q = 1, 2, 3),$$

with

$$k_{\pm q} = \sum_{\text{Hadrons } j \text{ with } S_j = \pm q} \tilde{n}_j V \quad (q = 1, 2, 3). \quad (2.5)$$

The canonical correction thus amounts to a multiplicative factor given by the ratio of the partition function with the strangeness of the considered hadron excluded to the complete partition function. This correction factor depends strongly on the volume,  $V$ , within which exact conservation is imposed. This correction factor rapidly approaches  $\lambda_S^S$  so that for most applications to heavy-ion collisions a grand-canonical treatment is sufficient.

While strangeness is exactly conserved in this ensemble, the baryon- and charge content is fixed only on average by the chemical potentials  $\mu_B$  and  $\mu_Q$  respectively.

### 3. The Canonical Ensemble

For small systems, such as  $pp$ ,  $p\bar{p}$ , and  $pA$  it is necessary to conserve each quantum number exactly [9, 10]. In such a system, with content  $B$ ,  $S$  and  $Q$ , the density, in the Boltzmann approximation, of hadron species  $i$  is

$$n_i^{B,S,Q}(T, B, S, Q, \gamma_S, V) = \left( \frac{Z_{B-B_i, S-S_i, Q-Q_i}}{Z_{B,S,Q}} \right) \tilde{n}_i(T, \mu = 0, \gamma_S), \quad (2.6)$$

where  $\tilde{n}_i$  is the associated density in the grand-canonical ensemble and  $Z_{B,S,Q}$  is the canonical partition function of the system. Calculation of the partition function has been performed by many groups (see references in [15]). In THERMUS the approach of [15] is adopted.

In this approach,

$$\begin{aligned} Z_{B,S,Q} &= \frac{Z_0}{(2\pi)^2} \int_0^{2\pi} d\phi_S \int_0^{2\pi} d\phi_Q \cos(S\phi_S + Q\phi_Q - B \arg \omega) \\ &\times \exp \left[ 2 \sum_{\text{Mesons } j} z_j^1 \cos(S_j\phi_S + Q_j\phi_Q) \right] I_B(2|\omega|), \end{aligned} \quad (2.7)$$

where,

$$\begin{aligned} \omega &\equiv \sum_{\text{Baryons } j} z_j^1 e^{i(S_j\phi_S + Q_j\phi_Q)}, \\ z_j^1 &\equiv \frac{g_j V}{(2\pi)^3} \int d^3 p e^{-E_j/T}, \end{aligned}$$

and  $Z_0$  is the total partition function of those hadrons with no net charges. Evaluation of the partition function involves labour-intensive numerical integration and is only practical in very small systems.

## B. Further Considerations

Although in the earlier discussion only expressions for the particle density were presented, the primordial energy and entropy densities and pressure are also easily determined from the appropriate partition function.

An essential ingredient in any thermal model analysis is a complete treatment of resonances. Especially at low temperatures it is important to take the width of these resonances into account. Resonance widths are included in the thermal model by distributing the resonance masses according to Breit-Wigner forms [2, 9, 10, 16, 17, 18]. This amounts to the following modification in the integration of the Boltzmann factor [17]:

$$\begin{aligned} &\int d^3 p \exp \left[ -\frac{\sqrt{p^2 + m^2}}{T} \right] \\ &\rightarrow \int d^3 p \int ds \exp \left[ -\frac{\sqrt{p^2 + s}}{T} \right] \frac{1}{\pi} \frac{m\Gamma}{(s - m^2)^2 + m^2\Gamma^2}, \end{aligned} \quad (2.8)$$

where  $\Gamma$  is the width of the resonance concerned, with threshold limit,  $m_{\text{threshold}}$ , and mass,  $m$ , and  $\sqrt{s}$  is integrated over the interval  $[m - \delta m, m + 2\Gamma]$ , where  $\delta m = \min[m - m_{\text{threshold}}, 2\Gamma]$ .

As input to the various thermal model formalisms one thus needs first a set of particles to be considered thermalised. When combined with a set of thermal parameters relevant to the ensemble under consideration, all primordial quantities (i.e. number density as well as energy- and entropy density and pressure) are calculable. Once the decays of each of the constituent hadrons is specified, the final particle densities can be determined and compared with experiment.

### III. IMPLEMENTATION IN THERMUS

Having briefly reviewed the thermal model we now discuss its implementation in THERMUS. The basic structure and functionality of THERMUS will be introduced by discussing the THERMUS classes in a bottom-up approach. The finer details of each class are discussed in the THERMUS manual available online (<http://hep.phy.uct.ac.za/THERMUS/>).

#### A. The Particle Object (TTMParticle)

The properties of a constituent of the hadron gas relevant to the thermal model are stored in a `TTMParticle` object. These properties include its mass, width, Monte-Carlo ID, degeneracy, statistics and quantum numbers. In addition, each `TTMParticle` object allows storage of the particle's decay channels in a list of `TTMDecayChannel` objects. Each of these elements of the list includes the branching ratio for the channel as well as the Monte-Carlo ID's of each of the daughters. From this decay channel list a decay summary list is generated in which each daughter appears only once.

#### B. The Parameter Set Object (TTMParameterSet)

The `TTMParameterSet` class is the base class from which the particular parameter set objects relevant to the individual varieties of thermal model implemented in THERMUS are derived (three at the moment). Each parameter set contains an array of `TTMParameter` objects which store the basic properties of a parameter (e.g. its name, value, error etc.).

The type of each parameter can also be specified. For instance, a parameter may be set to 'fit-type', if it is to be fitted, or 'constrained-type', if it is required that it be used to satisfy a certain constraint. These types refer to intended actions at this point; such action can only be taken at a later stage once the parameter set is combined with functions capable of implementing the intended actions. As an example, in grand-canonical treatments chemical potentials are often constrained by the initial conditions in the colliding system. However, such constraints can only be implemented once all densities in the hadron gas have been calculated.

#### C. The Thermal Particle Object (TTMThermalParticle)

Once a `TTMParticle` and `TTMParameterSet` object have been instantiated, these may be combined in a thermal particle object. The `TTMThermalParticle` class is the base class from which the three classes corresponding to the currently implemented varieties of the thermal model are derived.

Within the derived class relevant to a grand-canonical treatment of  $B$ ,  $S$  and  $Q$ , the parameters cannot yet be constrained (since a complete particle set is required for this). However, with the parameter values as specified, the particle-, energy- and entropy densities as well as the pressure are calculable. These quantities can be calculated assuming Boltzmann or Fermi-Dirac statistics, with or without resonance width.

The derived classes relevant to the two ensembles imposing exact conservation contain just calculations within the Boltzmann approximation. As we have seen, under this approximation, the thermal quantities are related to the grand-canonical quantities through correction factors. These factors, however, can only be calculated once a full set of hadronic constituents has been specified. At this level, with just one particle and a parameter set, the particle's correction factor has to be specified by the user. This structure was, however, maintained in order to allow analogous implementation of all formalisms at the `TTMThermalModel` level.

Although the Boltzmann no-width approximation leads to analytic results for all of the thermal quantities, all other calculations require numerical computation. In order to keep computation time reasonable, whenever possible, the Gauss-Laguerre quadrature method is used for the momentum integrals required under the assumption of quantum statistics and the Legendre method for the integrals required under the assumption of finite resonance width. A systematic test of these integration techniques has been conducted. In regions where these methods fail, the more labour-intensive `TF1` and `TF2` functions of `ROOT` are used. In practise, the more time-efficient algorithms work in most physical situations.

#### D. The Particle Set Object (`TTMParticleSet`)

The `TTMParticleSet` object contains a hash table of `TTMParticle` objects. The Monte-Carlo particle ID's are used to access these hadronic constituents quickly and efficiently from the set.

Associated with a particle set is a list of stable particles. In the context of the application of a thermal model, these are either particles which decay some time after reaching the detectors, or particles whose decays have been corrected for by the experimentalists. Once this list of stable particles is specified, the feed-down contributions to just these stable daughters are calculated and recorded in the decay summary list of each constituent. This allows for fast calculation of the feed-down contributions without continual re-calculation of the decay fractions to stable hadrons. By leaving the decay channel lists unaltered, this is not achieved at the cost of loss of information. Maintaining the decay channel information allows the possibility to extend `THERMUS` at a later stage to include also thermal freeze-out analysis of momentum spectra.

Although users are able to build their own particle sets, the `THERMUS` distribution contains a text file listing all hadrons with  $u$ ,  $d$  and  $s$  quarks listed by the Particle Data Group [19], as well as text files listing the particle decay channels. Using these files is the easiest way to instantiate a `TTMParticleSet` object and populate the decay lists of its constituents.

#### E. The Thermal Model Object (`TTMThermalModel`)

Combining a `TTMParticleSet` and `TTMParameterSet` object one can form a `TTMThermalModel` object. Derived classes exist for each of the previously discussed formalisms.

At this level, chemical potentials can be successfully constrained and canonical correction factors can be calculated, since all hadronic constituents and parameters are specified. Running `GenerateParticleDens` calculates all primordial particle densities after first automatically constraining the chemical potentials if required or calculating the canonical correction factors if relevant. If a particle is considered stable then a decay contribution is calculated based on the decays in the individual `TTMParticle` objects. These particle densities are stored in a hash table of `TTMDensObj` objects. Objects of this class allow storage of all thermodynamic quantities of a particle. Again access to the elements in this hash table is through the Monte-Carlo ID's.

Functions to calculate the energy and entropy densities and pressure of each particle also exist, but since they depend on the correction factors and chemical potentials determined from the particle densities, these functions must be run after `GenerateParticleDens`. When called, these functions cycle through the existing elements of the density hash table and insert the required quantity into each `TTMDensObj` object.

## F. The Thermal Fit Object (TTMThermalFit)

Since experimental groups frequently apply different feed-down corrections to particles, the `TTMThermalModel` class is not sufficiently flexible to allow fits to data. Instead a separate `TTMThermalFit` class has been developed with derived classes for each of the three formalisms. In these classes it is possible to ascribe to each particle yield or ratio of interest a particle set (or separate sets for the numerator and denominator in the case of ratios) with a different decay chain. In this way, feed-down chains can be fine-tuned to match the specifics of a particular experimental result. The yields or ratios of interest are stored as `TTMYield` objects in a list. Each `TTMYield` object contains the Monte-Carlo ID of the yield (or numerator and denominator ID's in the case of a ratio) as well as a further descriptive string. In addition to these identifiers, each `TTMYield` object includes a pointer (or pointers) to the relevant particle set (or sets), as well as the experimental and model values and errors.

The function `GenerateYields` cycles through the list and generates model predictions for each of the yields or ratios of interest based on the given parameter set and relevant particle sets.

The `FitData` function performs a fit of those parameters in the associated `TTMParameterSet` object of 'fit-type'. Use is made of the ROOT `TMinuit` fitting class. On completion of the fit, the parameter set contains the best-fit parameters and the list of yields and ratios of interest are populated with the best-fit model predictions.

## IV. CONCLUSION

In conclusion, an analysis package has been developed allowing thermal model analyses to be performed within the ROOT framework of analysis. This package is available freely from <http://hep.phy.uct.ac.za/THERMUS/>. A detailed user guide and installation instructions are also available at this site.

Subsequent to developing this package, the authors of THERMUS became aware of the release of a statistical hadronisation package (SHARE) written in FORTRAN and *Mathematica* [20]. THERMUS, however, has the advantage of being written for incorporation into ROOT.

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