

# Nonequilibrium phenomenology of identified particle spectra in heavy-ion collisions at energies available at the CERN Large Hadron Collider

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We employ the Zubarev approach of the statistical operator to investigate the enhancement of the low- $p_T$  region of pion spectra, introducing an effective pion chemical potential, to describe the overpopulation of low-energy pion states. We test a corresponding freeze-out approach by analyzing the transverse-momentum spectra of identified particles measured recently with high precision by the ALICE Collaboration in Pb + Pb collisions at CERN LHC. A blast-wave model and a blast-wave-based particle generator, coupled to a hadronic transport model, are utilized. Bayesian inference methods are applied to extract the most probable sets of thermodynamic parameters at the chemical freeze-out hypersurface. Both models for the overpopulated pion states, the hadronic transport model and the thermal model with a nonzero pion chemical potential, provide a satisfactory description of the observed pion spectra. However, both approaches contain approximations which can be improved within a systematic nonequilibrium approach. We demonstrate that the introduction of a nonequilibrium pion chemical potential offers an efficient alternative to the conventional explanation of the low- $p_T$  enhancement, typically attributed to resonance decays with subsequent thermalization. A similar discussion also holds for the kaon spectra.

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## I. INTRODUCTION

Since the early days of ultrarelativistic heavy-ion collisions (HIC) at CERN-SPS, the yields and spectra of identified particles have been the key observables to deduce the thermodynamic properties of the state of matter that has been created in these collisions [1]. In order to understand the emergence of hadronic yields, it has been expected that a statistical description following Hagedorn [2,3] could be applicable. Later it was demonstrated that the ratios of particle yields from the first CERN-SPS experiments could nicely be described within a simple chemical freeze-out model from the statistical equilibrium state of a hadron resonance gas with just two parameters, the freeze-out temperature and freeze-out baryon chemical potential [4]. However, as a caveat of such a statistical model of hadron production, the spectra of pions (and kaons) at low transverse momenta could not be described well with simple thermal distribution functions [5,6]. Compared with these distribution functions, the low- $p_T$  region of observed pion spectra are overpopulated.

A nonequilibrium distribution function with a finite pion (and kaon) chemical potential could well describe the observed enhancement in the low transverse-momentum part of the spectrum as a precursor of Bose-Einstein condensation [6]. Alternatively, the feed-down from resonance decays and the effect of radial flow has been considered [7] and gave at that time a satisfactory description of the spectra, which afterwards has been adopted as a standard tool in the theoretical description of particle spectra.

With the advent of high-precision and high-statistics data of identified particle production from the ALICE experiment at CERN-LHC [8,9], the problem of a precise description of the low-momentum pion spectra came up again since the modern hydrodynamic codes systematically underestimate the pion yield at low transverse momentum [10–12].

The same problem is present in the blast-wave fits of the experimental data and the simple feed-down from resonance decays is insufficient [8,13]. As a possible explanation, the critical enhancement of soft pions by fluctuations at the chiral transition [14] was proposed. Although the estimated enhancement factor agrees with the observed values, a direct comparison with the data was never performed. Another explanation was given in the framework of the nonequilibrium statistical-hadronization model with quark fugacity factors [15]. A blast-wave model combined with resonance decays was introduced in Ref. [16], while Ref. [17] employed a hydrodynamic simulation followed by a hadronic stage

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modeled under the assumption of partial chemical equilibrium (PCE), and then included resonance decays. Despite their advancements, the approaches mentioned before have significant limitations. In particular, Refs. [15] and [16] neglect hadronic rescatterings and final-state interactions, which are known to strongly modify particle spectra, resonance yields, and femtoscopic observables, and are essential for a consistent description of the data [18,19]. On the other hand, Refs. [13] and [17] include hadronic rescatterings but rely on the PCE assumption, which has been shown to fail in reproducing the resonance yields observed at LHC [20] and fails to reproduce the transverse-momentum spectra and mass dependence of the elliptic flow [21]. These findings suggest that the new high-precision CERN-LHC data requires a more fundamental and dynamically consistent description of the late-stage hadronic evolution, and can be understood by the inclusion of an out-of-equilibrium final hadronic stage right after hadronization.

In this work, we present a systematic nonequilibrium approach to pion production within the Zubarev method of the nonequilibrium statistical operator (NSO) [22] and apply it to a description of recent experimental data presented by the ALICE Collaboration [8,9]. To this end, we will develop and use a generalized blast-wave model and discuss different approximations, such as the introduction of a nonequilibrium chemical potential, and include also the effects of radial flow, resonance decays, and final-state interactions.

## II. THE METHOD OF NONEQUILIBRIUM STATISTICAL OPERATOR (NSO)

To describe the nonequilibrium processes of expanding hot and dense matter, the nonequilibrium statistical operator (NSO)  $\hat{\rho}$  is required, and the averages of the observables  $O$  are given by

$$\langle \hat{O} \rangle = \text{tr}\{\hat{\rho} \hat{O}\}. \quad (1)$$

The NSO  $\hat{\rho}$  is the solution of the Liouville–von Neumann equation, where the boundary conditions are given by the known averages of a set  $\{B_i\}$  of observables in the past [22]. According to Zubarev, the (information) entropy is introduced as the maximum of

$$S_{\text{inf}}[\hat{\rho}] = -\text{tr}\{\hat{\rho} \ln(\hat{\rho})\} \quad (2)$$

for given average values  $\langle \hat{B}_i \rangle$ . The solution, the relevant statistical operator  $\hat{\rho}_{\text{rel}}$ , can be used to formulate the boundary conditions for the solution of the Liouville–von Neumann equation [22].

In order to derive generalized equations of quantum relativistic hydrodynamics, a covariant formulation of the Zubarev NSO method can be given [23,24]. For this purpose, three-dimensional (3D) spacelike hypersurfaces  $\Sigma(\tau)$  are introduced depending on the parameter  $\tau$ , which does not necessarily coincide with the proper time marked by comoving clocks. The problem of different frames (Landau versus Eckart) was solved by Becattini *et al.* [25,26], see also Refs. [27–29], which give a recent overview of this (D.N. Zubarev called it “beautiful”) approach to quantum relativistic hydrodynamics.

We follow the work of Becattini *et al.* [26] and repeat some essential relationships. Similar to equilibrium, globally conserved quantities are of relevance to characterize the state of the system. In hydrodynamics, the energy-momentum density as well as the densities of other conserved quantities such as charge or particle number are of relevance. The mean values of energy-momentum and charge (or particle-number) density, calculated with  $\hat{\rho}_{\text{rel}}$ , should coincide with the actual values. We introduce the normalized timelike vector  $n_\mu(x)$  perpendicular to the hypersurface  $\Sigma$  and have

$$\begin{aligned} n_\mu(x) \langle \hat{T}^{\mu\nu}(x) \rangle &= n_\mu(x) \langle \hat{T}^{\mu\nu}(x) \rangle_{\text{rel}}, \\ n_\mu(x) \langle \hat{j}^\mu(x) \rangle &= n_\mu(x) \langle \hat{j}^\mu(x) \rangle_{\text{rel}}. \end{aligned} \quad (3)$$

The left-hand side of the above equation is calculated with a true state  $\hat{\rho}$  of the system, and the right-hand side is calculated with the relevant statistical operator  $\hat{\rho}_{\text{rel}}$ , which now depends on the chosen spacelike hypersurface  $\Sigma(\tau)$ , i.e., on the parameter  $\tau$ .  $\hat{T}^{\mu\nu}(x)$  denotes the (renormalized) operator of the energy-momentum tensor.  $\hat{j}_c^\mu(x)$  denotes the current density vector of the conserved component  $c$  [26].

The relevant statistical operator reads

$$\begin{aligned} \hat{\rho}_{\text{rel}} = Z_{\text{rel}}^{-1} \times \exp \left( - \int_{\Sigma} d\Sigma n_\mu(x) \left[ \beta_\nu(x) \hat{T}^{\mu\nu}(x) \right. \right. \\ \left. \left. - \sum_c \zeta_c(x) \hat{j}_c^\mu(x) \right] \right), \end{aligned} \quad (4)$$

where  $Z_{\text{rel}}$  is the normalization factor that makes  $\text{tr}\{\hat{\rho}_{\text{rel}}\} = 1$ . The vector  $\beta_\nu(x)$  and the scalar  $\zeta_c(x)$  are Lagrange parameters to be determined by solving the consistency relations (3). This special form of the relevant statistical operator  $\hat{\rho}_{\text{rel}}$  is also called local thermodynamic equilibrium,  $\hat{\rho}_{\text{LE}}$ . We can substitute  $\beta_\nu(x) = u_\nu(x)/T(x)$ ,  $\zeta_c(x) = \mu_c(x)/T(x)$ , where  $u_\nu(x)$  is the hydrodynamical four-velocity,  $u_\nu(x)u^\nu(x) = 1$ ,  $T(x)$  is the local temperature, and  $\mu_c(x)$  is the local chemical potential. These nonequilibrium generalizations of temperature, velocity, and chemical potentials are defined by the equations (3), but the solution of these equations, which can be regarded as nonequilibrium generalization of the equilibrium equations of state, is a difficult mathematical problem.

If we take  $n^\mu(x) = u^\mu(x) = (1, 0)$  and  $T, \mu_c = \text{const.}$ , we have

$$\begin{aligned} \int_{\Sigma} d\Sigma \left[ n_\mu(x) \frac{u_\nu(x)}{T(x)} \hat{T}^{\mu\nu}(x) \right] &= \frac{1}{T} \hat{H}, \\ \int_{\Sigma} d\Sigma \left[ n_\mu(x) \frac{\mu_c(x)}{T(x)} \hat{j}_c^\mu(x) \right] &= \frac{\mu_c}{T} \hat{N}_c, \end{aligned} \quad (5)$$

where  $\hat{H}$  is the Hamiltonian. For such a comoving system, the solution of the equations of consistency (3) can be performed using standard methods of quantum statistics. Such an approach is often used for the sake of calculational convenience. As is well known, the formation of bound states, the introduction of a wave function, and other many-particle effects is a difficult task within a covariant formalism, see Ref. [24]. We give a brief overview of the formalism in the comoving system. The original Zubarev NSO method is obtained by using Cartesian coordinates and hyperplanes as hypersurfaces

[26]. We use this formulation in a comoving system to make the physics more transparent.

To determine the statistical operator  $\hat{\rho}(t)$  for a nonequilibrium process, we have to solve the Liouville–von Neumann equation

$$\frac{\partial}{\partial t} \hat{\rho}(t) = \frac{i}{\hbar} [\hat{H}, \hat{\rho}(t)] \quad (6)$$

with given initial conditions (for the relativistic von Neumann equation see Ref. [24]). These initial conditions are represented by the average values of a set of relevant observables  $\{B_i\}$  in the past  $t' \leq t$ , which characterize the state of the system. This information is used to construct the relevant statistical operator  $\hat{\rho}_{\text{rel}}(t')$  as the maximum of information entropy

$$S_{\text{inf}}(t') = -\langle \ln[\hat{\rho}_{\text{rel}}(t')] \rangle_{\text{rel}} \quad (7)$$

under given constraints, the self-consistency conditions

$$\langle \hat{B}_i \rangle^{t'} = \text{tr}\{\hat{\rho}_{\text{rel}}(t') \hat{B}_i\}. \quad (8)$$

As well known from equilibrium statistics, these self-consistency conditions are taken into account via Lagrange parameters  $\lambda_i(t')$ , and we obtain the generalized Gibbs distribution

$$\hat{\rho}_{\text{rel}}(t') = \frac{e^{-\sum_i \lambda_i(t') \hat{B}_i}}{\text{tr}\{e^{-\sum_i \lambda_i(t') \hat{B}_i}\}}. \quad (9)$$

The Lagrange parameters  $\lambda_i(t')$  must be eliminated using the self-consistency conditions (8), which are the nonequilibrium generalizations of the equations of state. To obtain the equations of hydrodynamics, the operators  $\hat{B}_i$  and the Lagrange parameters  $\lambda_i$  can depend on position  $\mathbf{r}$  in addition to  $t'$ , see Zubarev *et al.* [22].

As already mentioned with respect to Eqs. (3), the solution of Eq. (8) is not trivial since the relevant operators can contain few-particle terms like the interaction in the Hamiltonian. We can apply many-particle techniques. A spectral function can be introduced; perturbation theory with respect to the interaction in the Hamiltonian gives the excitations of the system including the medium effects. For instance, the resonance gas represents a simple approximation. Note that a systematic approach requires the account of in-medium effects and continuum correlations, as needed, for instance, to explain the high-precision data for the yields measured in the ALICE experiment [30,31].

Below we discuss the density as relevant observable, depending on temperature  $T$  and chemical potentials  $\mu_c$ , Eq. (5). We mention three approximations to solve (8), i.e., to treat the spectral function: (i) the ideal quantum gas, (ii) the resonance-gas approximation where excited states are treated in chemical equilibrium, and (iii) the inclusion of in-medium effects such as the quasiparticle shifts, Pauli blocking, continuum correlations as known from the generalized Beth-Uhlenbeck formula [32], and the description of the Mott effect for clusters [33].

The solution of the Liouville–von Neumann equation at given boundary conditions (8) is [22]

$$\hat{\rho}(t) = \lim_{\epsilon \rightarrow 0} \epsilon \int_{-\infty}^t dt' e^{-\epsilon(t-t')} e^{-\frac{i}{\hbar} \hat{H}(t-t')} \hat{\rho}_{\text{rel}}(t') e^{\frac{i}{\hbar} \hat{H}(t-t')}. \quad (10)$$

Having  $\hat{\rho}(t)$  to our disposal, we can follow the time evolution of the system. In particular, we can calculate transport coefficients (reaction rates) [22]. Within a quantum-statistical approach, in simplest approximation the free-reaction rates are obtained. Improved approximations lead to medium modifications of the transport coefficients, see, for example, Ref. [34].

A particular problem of the NSO method is the selection of the set of relevant observables  $\{B_i\}$ . We have to consider long-living fluctuations because they need a long time to be built up dynamically and demand higher orders of perturbation theory. A minimum set of relevant observables consists of the conserved quantities: energy  $H$  as well as the conserved numbers  $N_i$ . The Gibbs distribution

$$\hat{\rho}_{\text{rel}}(t) \propto \exp \left[ -\left( \hat{H} - \sum_i \lambda_i(t) \hat{N}_i \right) / \lambda_T(t) \right] \quad (11)$$

contains the Lagrange multipliers  $\lambda_i(t)$ ,  $\lambda_T(t)$  which are, in general, time dependent. They are not identical to the equilibrium parameters temperature and chemical potentials, but can be regarded as their generalizations in nonequilibrium.

If the relaxation time  $\tau_r$  of any fluctuation in the state described by  $\hat{\rho}_{\text{rel}}(t)$  is short, the limit  $\epsilon \rightarrow 0$  in Eq. (10) can be replaced by  $\epsilon \leq 1/\tau_r$ , the memory of the system is short (Markov limit). Then,  $\hat{\rho}(t)$  can be replaced by  $\hat{\rho}_{\text{rel}}(t)$  and the time evolution of the system is described by the relevant distribution, with fluctuations  $B_i$  for which  $\dot{\lambda}_i/\lambda_i \leq 1/\tau_r$  should be considered as new relevant observables. The relevant distribution based on the former set  $\{B_i\}$  of relevant observables freezes out if the processes which change the distribution slow down (see Appendix). The temporary evolution of the system in Markov approximation requires a larger set of relevant observables which includes the slow observables  $B_l$ . For instance, the occupation numbers of single-particle states may be included to obtain reaction-kinetic equations for the distribution function describing the evolution of the system after (chemical) freeze-out of the thermodynamic equilibrium. For more details with respect to the NSO method, see Appendix.

In this work, we do not study the time evolution of the nonequilibrium Lagrange multipliers  $\lambda_i(t)$  and  $\lambda_T(t)$ , but infer their values on the chemical and kinetic freeze-out hypersurfaces using the model described in the next section. For simplicity, we refer to these values as  $\lambda_i(t_{\text{freeze}}) = \mu_i$  and  $\lambda_T(t_{\text{freeze}}) = T$  in the following. Our main contribution is a systematic phenomenological comparison and a framework-motivated parametrization, rather than implying a fully dynamical NSO-based description of the hadronic stage.

### III. BLAST-WAVE MODEL OF PARTICLE FREEZE-OUT

To describe the system formed in a heavy-ion collision, one must consider the fast system expansion. However, instead of introducing the collective velocity as another relevant

TABLE I. Approximations corresponding to the models A–D for describing particle production in HIC, (i)–(iii) concern the treatment of the spectral function (8), for details see text.

| Model | Approximations       |         |         |           |         |                             |                     |                             |                            |
|-------|----------------------|---------|---------|-----------|---------|-----------------------------|---------------------|-----------------------------|----------------------------|
|       | Lagrange multipliers |         |         |           |         | Kinetic                     |                     |                             | Final                      |
|       | $T$                  | $\mu_p$ | $\mu_n$ | $\mu_\pi$ | $\mu_K$ | (i)<br>Ideal<br>$p, \pi, K$ | (ii)<br>Res.<br>gas | (iii)<br>In-med.<br>effects | Decays<br>+<br>scatterings |
| A     | ✓                    | ✓       | ✓       | –         | –       | –                           | –                   | –                           | –                          |
| B     | ✓                    | ✓       | ✓       | ✓         | ✓       | –                           | –                   | –                           | –                          |
| C     | ✓                    | ✓       | ✓       | –         | –       | ✓                           | ✓                   | –                           | ✓                          |
| D     | ✓                    | ✓       | ✓       | ✓         | –       | ✓                           | ✓                   | –                           | ✓                          |

observable and deriving the hydrodynamic equations from the NSO [28], we employ the blast-wave model parametrization in its standard form [7], assuming that particles are emitted from the boost-invariant and cylindrically symmetric hypersurface  $\Sigma_\mu$  with the volume element  $d\Sigma_\mu$  given by

$$d\Sigma_\mu = (\tau r \cosh \eta, 0, 0, -\tau r \sinh \eta) dr d\phi d\eta, \quad (12)$$

at a constant value of the proper time  $\tau = \sqrt{t^2 - z^2} = \text{const.}$  Here  $r$  is the transverse radius,  $\phi$  is the azimuthal angle in coordinate space, and  $\eta = \tanh^{-1}(z/t)$  is the space-time rapidity. In this model,  $r \in [0; R]$  and  $\eta \in [-\eta_{\max}; \eta_{\max}]$ , with  $R$  and  $\eta_{\max}$  being the system size in transverse and longitudinal directions, respectively. The collective flow velocity in midrapidity is parametrized as

$$u^\mu(r, \eta = 0) = (\cosh \rho, \sinh \rho \cos \phi, \sinh \rho \sin \phi, 0), \quad (13)$$

where  $\rho$  is the velocity profile

$$\rho = \tanh^{-1} \left[ \beta_s \left( \frac{r}{R} \right)^n \right], \quad (14)$$

$$\frac{d^6 N_i}{dp_T dy d\eta dr d\phi d\psi} = \frac{g_i \tau r p_T m_T}{(2\pi \hbar)^3} \cosh(y - \eta) \left( \exp \left[ \frac{m_T \cosh \rho \cosh(y - \eta) - p_T \sinh \rho \cos(\phi - \psi) - \mu_i}{T} \right] + a_i \right)^{-1}, \quad (17)$$

where  $p_T$  is the transverse momentum of the particle,  $m_T$  the transverse mass of the particle,  $\psi$  is the azimuthal angle in momentum space, and  $y$  is the rapidity of the particle.

For resonances, we include additional mass attenuation in the form of the nonrelativistic Breit-Wigner distribution with constant width. Since particle-antiparticle ratios in the energy range of interest are approximately unity over a broad transverse-momentum range, we set baryon, strangeness, and electric-charge chemical potentials to zero. This reduces the number of free parameters while maintaining a reasonable fit quality. Then the particle chemical potential is defined as

$$\mu_i = \mu_\pi \delta_{i,\pi} + \mu_K \delta_{i,K}, \quad (18)$$

where  $\mu_\pi$  and  $\mu_K$  are pion and kaon nonequilibrium effective chemical potentials. The model's program code can be found at Zenodo [36].

with the profile exponent  $n$  and transverse expansion velocity at the surface  $\beta_s$ . The full velocity field is obtained by boosting Eq. (13) in the  $\eta$  direction. Having the freeze-out hypersurface and collective velocity fields defined, the particle invariant-momentum distribution is given by the Cooper-Frye formula [35]:

$$E \frac{d^3 N_i}{d^3 p} = \frac{g_i}{(2\pi \hbar)^3} \int d\Sigma_\mu p^\mu f_i(p^\mu u_\mu), \quad (15)$$

where  $g_i$  is the spin-degeneracy factor of the  $i$ th particle species,  $p_\mu$  is the particle four-momentum, and  $f_i(E)$  is the particle distribution function

$$f_i(E) = \left( \exp \left[ \frac{E - \mu_i}{T} \right] + a_i \right)^{-1}, \quad (16)$$

with  $a_i = +1$  for fermions and  $a_i = -1$  for bosons, and  $\mu_i$  and  $T$  being the particle chemical potential and freeze-out temperature or their nonequilibrium generalizations from the NSO method if nonequilibrium is assumed. Then the resulting particle distribution function is given as

#### IV. RESULTS AND DISCUSSION

To solve the puzzle of the low-momentum enhancement of the pion spectra in HIC at ultrarelativistic energies [37] we apply the method of the NSO. We can include the numbers  $N_\pi$  and  $N_K$  of pions/kaons into the set of relevant variables since they are long-living fluctuations, with lifetimes determined by weak interaction.

Different approximations are considered (see Table I): Model A is the standard blast-wave model without hadron resonances and their decays, no final-state rescattering applied for the description of pion, kaon, and proton spectra at the kinetic freezeout, see Fig. 1. A strong deviation from ALICE data at low momenta is observed. The conventional approximation A gives similar results to those reported in the ALICE publication [8]. Namely, the temperature is about 95 MeV, and the surface velocity is about 87% of the speed of light.

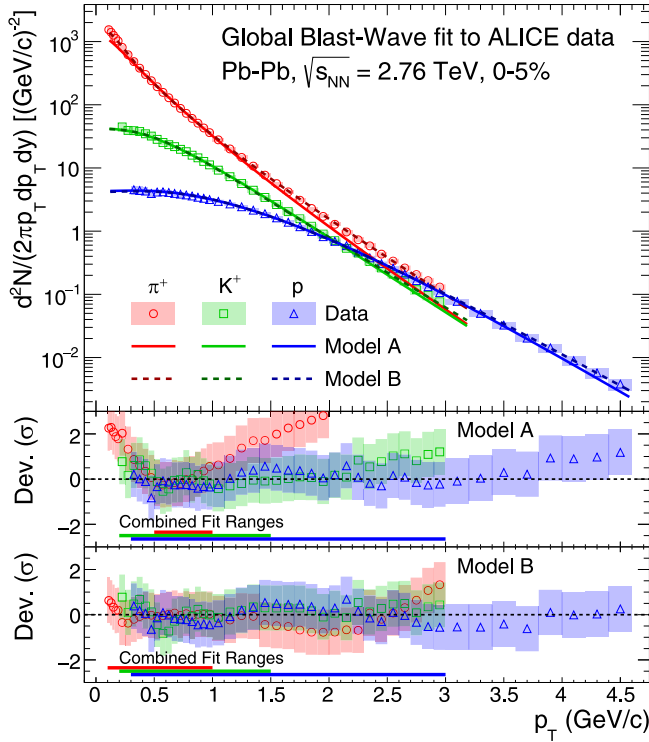


FIG. 1. Transverse-momentum spectra of  $\pi^+$ ,  $K^+$ , and  $p$  (antiparticles are not shown) measured by the ALICE collaboration [8] in 0–5% central PbPb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV compared to the standard blast-wave fit and to the fit with nonequilibrium distribution function.

In model B, we introduce the pion and kaon chemical potentials  $\mu_\pi$  and  $\mu_K$  into the Bose distribution [6,38] which enters the blast-wave function (17). The fit result is shown in Fig. 1 and the fit parameters are summarized in Table II. Compared to model A, the fit gives a significantly higher temperature, i.e., about 120 MeV at roughly the same flow velocity. The pion and kaon chemical potentials are high and close to the particle masses with  $\mu_\pi = (126.2 \pm 3.8)$  MeV and  $\mu_K = (402.9 \pm 22.6)$  MeV. Similar results have been obtained in Refs. [6,39,50]. One can see that such an extension gives not only the correct pion/kaon particle density but also the spectra using just two additional parameters. Our extraction of the effective pionic chemical potential is significantly higher than expectations from theory, see Refs. [39–41]. Such a discrepancy might suggest that the hadronized matter is not

produced with  $\mu_\pi = 0$  if  $\mu_\pi$  is to rise to the level we suggest by the time the matter disassociates.

The blast-wave function (17) is fitted to the data by minimizing the  $\chi^2$  over the combined fit range. Following the experimental procedure [8,37,42], for model A we set the combined fit  $p_T$  ranges to 0.5–1.0 GeV/c for  $\pi^\pm$ , 0.2–1.5 GeV/c for  $K^\pm$ , and 0.3–3.0 GeV/c for (anti-)protons [8]. For model B to be sensitive to changes in  $\mu_\pi$ , we extend the  $p_T$  fit range for  $\pi^\pm$  to 0.1–1.0 GeV/c. To examine the overall fit quality, we introduce  $\chi^{2*}$ , which is the  $\chi^2$  function evaluated for all spectra over the  $p_T \in [0, 2]$  GeV/c. It is remarkable that the fit with model B describes the data over a broad  $p_T$  range, even outside of the fit ranges, since  $\chi^{2*}$  is 6.7 times better in the extended model with finite effective chemical potentials than in model A. The NSO-based approximation B with pion and kaon chemical potentials provides an excellent description of the particle spectra including the low-momentum enhancement.

In the approximations C and D of Table I, we explicitly account for resonance decays and final-state interactions between hadrons. This is an attempt to extend the description of the system to a stage before the kinetic freeze-out, namely, to the chemical freeze-out stage. For this purpose, we developed a blast-wave-based thermal particle generator coupled with the SMASH hadronic transport model [43]. First, for a given set of model parameters, we sample the particles' positions, momenta, and, for unstable states, masses on the freeze-out hypersurface using the previously obtained distribution function (17). We use all hadronic states from the SMASH particle list that do not contain charm and bottom quarks. Then, the particles generated from the freeze-out hypersurface are input into the SMASH model, which serves as an afterburner, performing resonance decays, elastic scatterings, and other final-state interactions. Taking into account the nonzero value of the effective pion chemical potential at kinetic freeze-out, we challenge the assumption of the chemical equilibrium on the hadronization surface and consider two cases: model C with full chemical equilibrium and model D with the overpopulated pion state, modeled by the inclusion of the effective pion chemical potential.

To infer the model parameters, we use the Bayesian-analysis workflow similar to the one used in Ref. [44]. Since the full model is computationally expensive, we replace it with Gaussian-process emulators and reduce the number of emulators needed using the principal component analysis. Uniform priors and multivariate normal likelihood were used in this analysis. The marginal posterior probability distributions of the model parameters were obtained using the Markov-chain

TABLE II. Results of the combined blast-wave fits of identified particle spectra at kinetic freeze-out (KFO) and the MAP estimate of the model parameters from the Bayesian analysis at the chemical freeze-out (CFO) with and without pion/kaon chemical potential.  $\tau$ ,  $R$ ,  $\beta_s$ ,  $n$  are parameters of the blast-wave model, Eq. (17).

| Model  | $\tau$ (fm/c) | $R$ (fm) | $T$ (MeV)       | $\beta_s$         | $n$               | $\mu_\pi$ (MeV) | $\mu_K$ (MeV)    | $\chi^2/\text{ndof}$ | $\chi^{2*}/\text{ndof}$ |
|--------|---------------|----------|-----------------|-------------------|-------------------|-----------------|------------------|----------------------|-------------------------|
| A) KFO | –             | –        | $97.7 \pm 3.9$  | $0.879 \pm 0.005$ | $0.709 \pm 0.019$ | –               | –                | 0.148                | 0.956                   |
| B) KFO | –             | –        | $118.1 \pm 3.7$ | $0.858 \pm 0.005$ | $0.662 \pm 0.023$ | $126.2 \pm 3.8$ | $402.9 \pm 22.6$ | 0.136                | 0.143                   |
| C) CFO | 8.88          | 11.54    | 154.02          | 0.786             | 0.699             | –               | –                | 0.1                  | 0.1                     |
| D) CFO | 8.08          | 11.5     | 155.98          | 0.783             | 0.697             | 9.52            | –                | 0.1                  | 0.1                     |

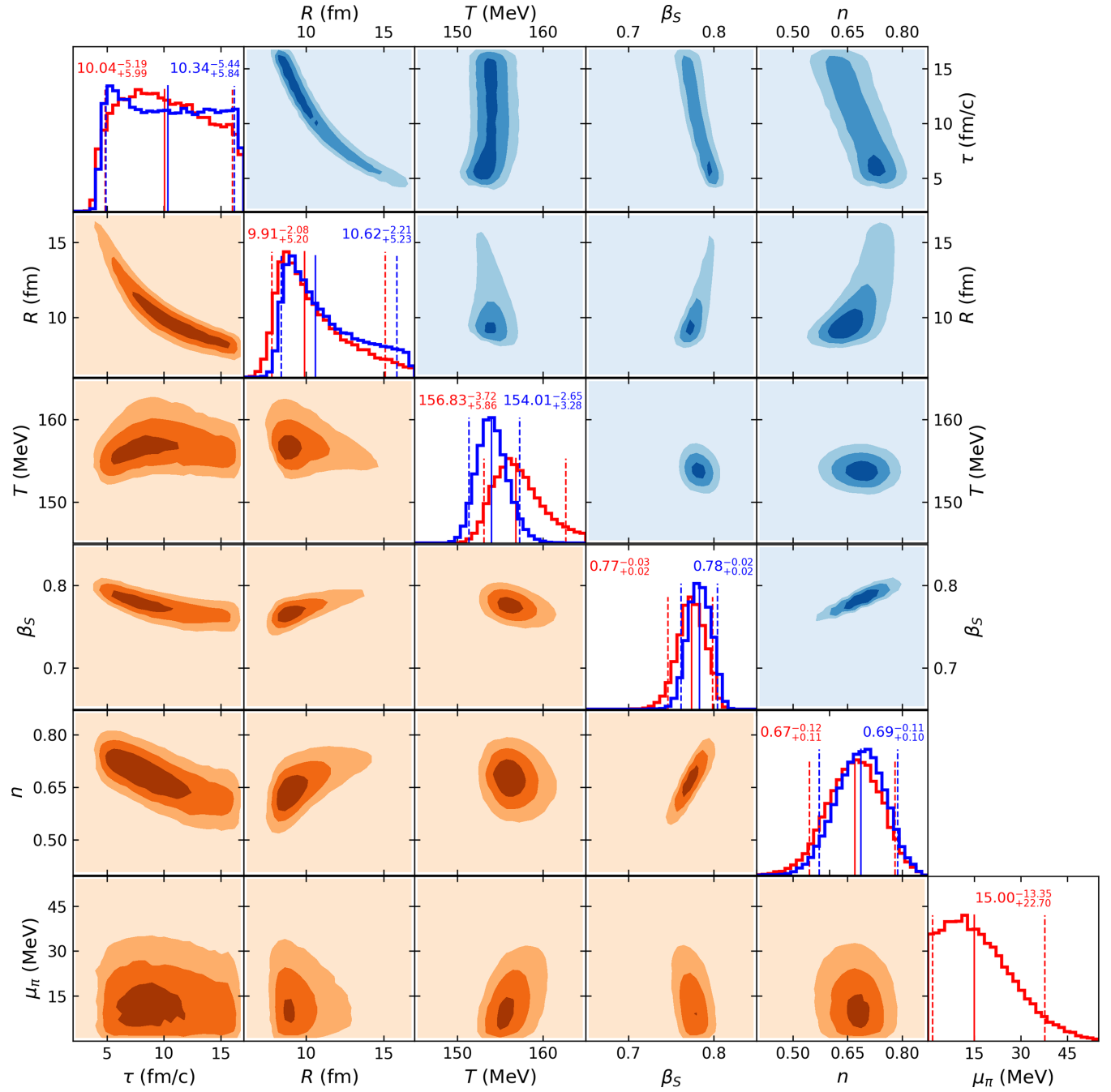


FIG. 2. Marginal (on diagonal) and joint-marginal posterior probability distributions of model parameters for model C (blue, upper triangle) and model D (orange, lower triangle) of the overpopulated pion states. Solid and dashed vertical lines and numeric values indicate median values and 90% credible intervals of the parameter distributions, respectively.

Monte Carlo sampling. They are shown in Fig. 2 together with the median values and 90% credible intervals; see also Table II for a maximum *a posteriori* probability (MAP) estimate of the parameter values. The transverse-momentum spectra for models C and D are shown in Fig. 3. Bayesian analysis using a blast-wave model coupled to SMASH gives a posterior temperature of about 156 MeV, which is consistent with the pseudocritical temperature found in lattice QCD simulations [45,46] and statistical hadronization models [47–49], and a mean flow velocity of about 77% of the speed of light.

Repeating the same analysis with model D results in the same fit quality and a value for  $\mu_\pi$  that is compatible with zero. This is confirmed by the fact that the corresponding Bayes factor [12]  $B_C^D = 0.434$  is of the order unity, while the posterior distributions for model D are getting broader, which is seen in Fig. 2.

We show that both models B and C describe the situation of the overpopulation of the low-momentum pion states, but in different approximations. After the chemical freeze-out, inelastic collisions between hadrons no longer contribute to the

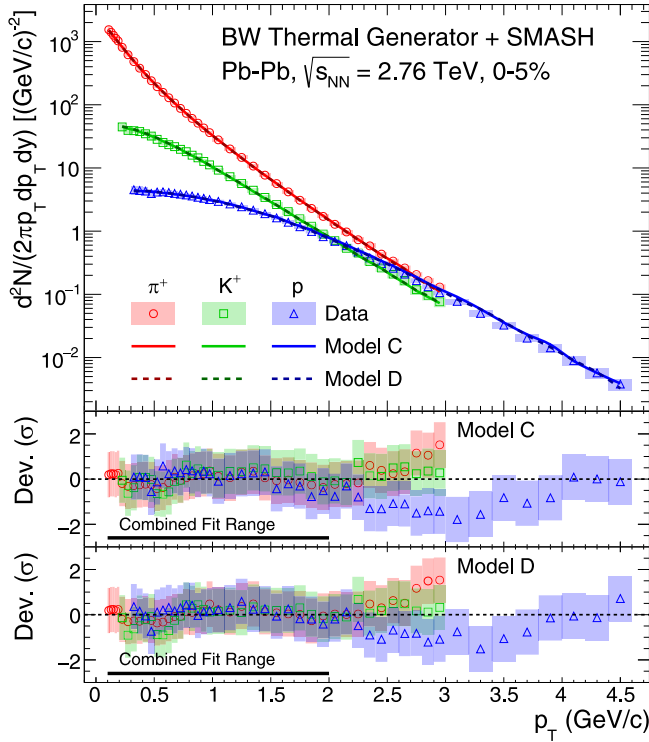


FIG. 3. Transverse-momentum spectra of pions, kaons, and protons (antiparticles are not shown) compared to the MAP estimate from models C and D.

changes in occupation numbers, while resonances still can decay and (quasi-)elastic processes lead to thermal equilibration and modify hadron spectra until kinetic freeze-out. During this stage, the effective number of pions/kaons remains nearly conserved in the sense that a hadronic resonance that decays into a number of pions may be regarded as a reservoir for that same number of additional pions [50]. Since pion/kaon decay is a weak process that is sufficiently slow, the pion number  $N_\pi$  and the kaon number  $N_K$  must be included in the set of relevant observables  $\{B_i\}$ . This leads to the appearance of the effective chemical potential  $\mu_i$  in the distribution function (17) as a consequence of the self-consistency condition (8). An explicit treatment of resonance decays and final-state interactions using SMASH confirms this result.

## V. CONCLUSIONS

In conclusion, models B, C, and D provide reasonable approximations to describe the dynamics of the expanding fireball. The model C offers a microscopic description of the collision processes and resonance decays including rescattering, albeit with free-space parameters without medium effects, starting at the chemical freeze-out surface and continuing through to kinetic freeze-out. The extension of the relevant distribution introducing the Lagrange parameter  $\mu_\pi$  in model D does not give essential improvement because the mesonic overpopulation at low  $p_T$  is already described by the decay of resonances and their thermalization. In contrast, model B reflects this overpopulation of low- $p_T$  meson states after

thermalization, without following microscopically the thermalization process. We emphasize that the physics driving the shape of the spectra at low  $p_T$  is from Bose symmetrization and that raising  $\mu_\pi$  tilts the spectra toward lower  $p_T$ . The results show that this simple extension of the blast-wave model with mesonic effective chemical potentials presents an efficient alternative for describing particle spectra at kinetic freeze-out. The simple model B can also be improved considering a better approximation of the spectral function evaluating Eq. (8) with the extended set of Lagrange parameters, taking into account correlations.

However, all models, in particular C and D, are also approximations since they do not consider in-medium effects, for instance the Mott effect [33], which are essential at high densities. To be consistent with the current calculations that explain the particle yields obtained from high-precision experiments [30,31], which explicitly show the role of in-medium corrections, an improved treatment of the spectra with in-medium corrections is also required, left for future work.

In a next step of the development of Zubarev's NSO approach to describe the nonequilibrium evolution of the hadron resonance gas created in heavy-ion collisions would be the extension of the set of observables (8) to include the flow of particle species and to describe the formation of resonances as a result of interactions to be included to the model Hamiltonian. The goal of such an extended NSO approach would be to provide a consistent scenario for hadron production in heavy-ion collisions which shall justify the success of the thermal statistical model and its limitations. To give an example, the fugacity parameters that are introduced in thermal statistical models on an *ad hoc* basis to improve the description of experimental data (see, e.g., Refs. [15,51]) could be related to the Lagrangian multipliers in the NSO formalism and would thus appear as the result of a consistent and systematic approach applied to describe the system.

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## DATA AVAILABILITY

The data that support the findings of this article are openly available [36].

## APPENDIX: THE ZUBAREV NSO METHOD

We discuss some details of the Zubarev NSO method as a general approach to treating a nonequilibrium system. Since our present work concerns only the application to heavy-ion collisions at high energies, some fundamental questions of the NSO method are discussed here separately.

A first question is whether Eq. (10) is a solution of the Liouville–von Neumann equation (6). Let us introduce instead of  $\hat{\rho}(t)$  [Eq. (10)] the quantity

$$\hat{\rho}_\epsilon(t) = \epsilon \int_{-\infty}^t dt' e^{-\epsilon(t-t')} e^{-\frac{i}{\hbar}\hat{H}(t-t')} \hat{\rho}_{\text{rel}}(t') e^{\frac{i}{\hbar}\hat{H}(t-t')}, \quad (\text{A1})$$

with a finite value of  $\epsilon$ . The expression  $\hat{\rho}(t)$  (10) follows in the limit  $\epsilon \rightarrow +0$ , which must be performed after the thermodynamic limit (van Hove limit), in which volume  $V \rightarrow \infty$ ,  $N/V$  is constant, so that the spectrum of energy eigenvalues of  $H$  becomes dense.

We easily find the equation

$$\frac{\partial}{\partial t} \hat{\rho}_\epsilon(t) - \frac{i}{\hbar} [\hat{H}, \hat{\rho}_\epsilon(t)] = -\epsilon [\hat{\rho}_\epsilon(t) - \hat{\rho}_{\text{rel}}(t)]. \quad (\text{A2})$$

Compared with the Liouville–von Neumann equation (6), on the right-hand side a source term appears which becomes zero in the limit  $\epsilon \rightarrow 0$ . In this sense,  $\hat{\rho}(t)$  (10) is a particular solution of the Liouville–von Neumann equation (6).

A more detailed discussion of the mathematical background (Abel's theorem) is found in the book of Zubarev [52]. Similarly to the Heisenberg ferromagnet, where an arbitrary small external magnetic field can be introduced to break the rotational symmetry, so that a magnetic moment can be formed, the infinitesimal small source term breaks the time-inversion symmetry, and the retarded solution of Eq. (6) is selected out. For a discussion of the source term in Eq. (A2) see also Röpke [53].

After integration by parts, the expression (A1) can be rewritten as

$$\begin{aligned} \hat{\rho}_\epsilon(t) &= \hat{\rho}_{\text{rel}}(t) + \int_{-\infty}^t dt' e^{-\epsilon(t-t')} e^{-\frac{i}{\hbar}\hat{H}(t-t')} \\ &\times \left\{ \frac{i}{\hbar} [\hat{H}, \hat{\rho}_{\text{rel}}(t')] - \frac{\partial}{\partial t'} \hat{\rho}_{\text{rel}}(t') \right\} e^{\frac{i}{\hbar}\hat{H}(t-t')}. \end{aligned} \quad (\text{A3})$$

This may be considered as the subdivision of  $\hat{\rho}(t) = \hat{\rho}_{\text{rel}}(t) + \hat{\rho}_{\text{irrel}}(t)$  in a relevant part and an irrelevant part, after the limit  $\epsilon \rightarrow +0$  has been performed.

Another question refers to the selection of the set of relevant observables  $\{B_n\}$ , see Eq. (8). This is the main problem of the present work. It must contain the conserved quantities; all other observables evolve dynamically, and according to the ergodic hypothesis, the full phase space is covered. However, there is no first-principle approach to select them since in the limit  $\epsilon \rightarrow +0$ , the source term in Eq. (A2) vanishes for any choice of the set  $\{B_n\}$ . It is of practical relevance to include all slow variables so that a quick relaxation to the corresponding  $\hat{\rho}_{\text{rel}}(t)$  takes place, and in the Markov approximation it is possible to treat the integral part of  $\hat{\rho}_\epsilon(t)$ . Different applications are considered in Röpke [54] where also the solution of the nonequilibrium equations of state (8) using the Green's function method is discussed.

Typical examples are linear-response theory where the system is near thermodynamic equilibrium, but also kinetic theory where the distribution function can be far from thermodynamic equilibrium, see also Zubarev *et al.* [22]. To give an example for the role of the irrelevant part of the statistical operator (A3), it is well known that within the Boltzmann kinetic theory, which was derived from the NSO according to the seminal work of Bogoliubov [55], only the kinetic energy is conserved, not the total energy as required. This problem arises because only the single-particle occupation numbers are considered as relevant observables, and the Markov approximation was performed.

This problem can be resolved considering the memory effects contained in  $\hat{\rho}_{\text{irrel}}(t)$ . Alternatively, we can include the Hamiltonian  $\hat{H}$  in the set of relevant observables  $\{B_n\}$  so that the simultaneous description of the many-particle system by hydrodynamics and kinetic theory is possible; see Zubarev *et al.* [56]. Processes which are hidden in the irrelevant part of the statistical operator are transferred to the relevant part, and the Markov approximation is then possible. This is also the main point in our approach where we introduce the chemical potentials of pions and kaons, so that the use of reaction kinetics as in the standard codes is improved.

The other item of our approach is the use of Green's function techniques to solve the nonequilibrium equations of state (8) so that in-medium density effects can be included. In the present work we only point out the relevance of the Mott effect but have not modified the quasiparticle energies and cross sections owing to medium effects in the reaction kinetic equations.

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