Using the Ultra-relativistic Quantum Molecular Dynamics (UrQMD) model to extract the thermal conductivity transport coefficient of hadron gas

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Abstract. The thermal conductivity of hadronic matter is studied using a microscopic transport model, which will be used to simulate ultra-relativistic heavy ion collisions at different energy densities ε, namely the Ultra-relativistic Quantum Molecular Dynamics (UrQMD). The molecular dynamics simulation is performed for a system of zero baryon number density and light meson species (π, ρ and K) in a box with periodic boundary conditions. The equilibrium state is investigated by studying the chemical equilibrium and the thermal equilibrium of the system. The particle multiplicity equilibrates with time, and the energy spectra of different light mesons species have the same slopes and common temperatures when thermal equilibrium is reached. The thermal conductivity transport coefficient is calculated from the heat current - current correlations using the Green-Kubo relations.

1. Introduction

A large number of studies in heavy ion physics and high energy physics have been done using the results from the Relativistic Heavy Ion Collider (RHIC). Now with the restart of the Large Hadron Collider (LHC) physics programme, the field of high energy nuclear physics, and especially heavy ion physics, has gone into a new era. It is now possible to explore the properties of Quantum-Chromo-Dynamics (QCD) at unprecedented particle densities and temperatures, and at much higher energies than that produced at RHIC, from $\sqrt{s} = 200$ GeV to $\sqrt{s} = 14$ TeV at the LHC [1].

High energy heavy ion reactions are studied experimentally and theoretically to obtain information about the properties of nuclear matter under extreme conditions at high densities and temperatures, as well as about the phase transition to a new state of matter, the quark-gluon plasma (QGP) [2, 3]. This work reports on a transport coefficient, namely the thermal conductivity of hadron matter. Other transport coefficients such as shear and bulk viscosity are well discussed and documented [3, 4], but the study of the thermal conductivity transport coefficient is poorly documented, especially with the use of UrQMD model to simulate ultra-relativistic heavy ion collisions. The knowledge of this transport coefficient plays an important role in the development of a model such as the UrQMD model, and also the development of high energy heavy ion experiments such as LHC and RHIC.

Equilibration of the system is studied by evaluating particle number densities from chemical equilibrium, energy spectra as well as the temperatures from thermal equilibrium of different light meson species in a cubic box, which imposes periodic boundary conditions. The infinite hadronic matter is modelled by initializing the system with light meson species namely, the pion (π), the rho (ρ) and the kaon (K). We focus on the hadronic scale temperature (100 MeV $< T <$ 200 MeV) and zero baryon number density, which are expected to be realized in the central high energy nuclear collisions [5]. We then change energy density from ε = 0.1 - 2.0 GeV/fm^3 and for each energy density we run the system with 200 events while keeping the volume and baryon number density constant until the equilibrium state is reached. The thermal conductivity transport coefficient is calculated from the heat current - current correlations using the Green-Kubo relations.

The rest of the paper is organized as follows: In section 2 we study the description of the UrQMD model. In section 3 we study equilibration properties of the system. In section 4 we calculate the thermal conductivity transport coefficient around the equilibrium state through the UrQMD model using Green-Kubo relations.

2. Short Description of the UrQMD Model

The Ultra-relativistic Quantum Molecular Dynamic model (UrQMD) is a microscopic model based on a phase space description of nuclear reactions. We use version 3.3 of the UrQMD model for this study. The UrQMD 3.3 hybrid approach extends previous ansatzes to combine the hydrodynamic and the transport models for the relativistic energies. The combination of these approaches into one single framework, it is done for a consistent description of the dynamics

The UrQMD model describes the phenomenology of hadronic interactions at low and intermediate energies from a few hundreds MeV up to the new LHC energy of $\sqrt{s}$ =14 TeV per nucleon in the centre of mass system [6, 7]. The UrQMD collision term contains 55 different baryon species and 32 meson species, which are supplemented by their corresponding anti-particles and all the isospin-projected states [6, 8]. The properties of the baryons and the baryon-resonances which can be populated in UrQMD can be found in [8], together with their respective mesons and the meson-resonances. A collision between two hadrons will occur if

$$d_{\text{trans}} \leq \sqrt{\frac{\sigma_{\text{tot}}}{\pi}}, \qquad \sigma_{\text{tot}} = \sigma(\sqrt{s}, type), \tag{1}$$

where d_{trans} and σ_{tot} are the impact parameter and the total cross-section of the two hadrons respectively [6]. In the UrQMD model, the total cross-section σ_{tot} depends on the isospins of colliding particles, their flavour and the centre-of-mass energy $\sqrt{s}$. More details about the UrQMD model is presented in [6, 7, 8].

3. Equilibration of Hadronic Matter

To investigate the equilibrition of a system, the UrQMD model is used to simulate the ultra-relativistic heavy ion collisions. A multi-particle production plays an important role in the equilibration of the hadronic gas [3]. The cubic box used for this study is initialised according to the following numbers of baryons and mesons: zero protons, 80 pions, 80 rhos and 80 kaons. For this study a cubic box with volume V and a baryon number density n_B = 0.00 fm^{-3} is considered. The energy density ε, volume V and the baryon number density n_B in the box are fixed as input parameters and are conserved throughout the simulation. The energy density is defined as $\varepsilon = \frac{E}{V}$, where E is the energy of N particles and the three-momenta p_i of the particles in the initial state are randomly distributed in the centre of mass system of the particles as shown in the equations below.

$$E = \sum_{i=1}^{N} \sqrt{m_i^2 + p_i^2}, \qquad \sum_{i=1}^{N} p_i = 0. \tag{2}$$

3.1. Chemical Equilibrium

In this subsection the chemical equilibrium is studied from the particle number densities of different light meson species in a box with V = 1000 fm^3, zero net baryon number density n_B = 0.0 fm^{-3} at different energy densities using UrQMD box calculations. Figure 1 (a) and (b) represents the time evolutions of the various meson number densities at $\varepsilon = 0.3$ and 0.4 GeV/fm^3 energy densities.

In figures 1 (a) and (b), the meson species indicate that the system does indeed reach chemical equilibrium. It is observed that the pions have large particle number densities and the reason could be the decay in the heavier mesons and other particles produced in the system to form pions. The saturation of the particle number densities indicate the realization of a local equilibrium. In conclusion, the chemical equilibrium of the system has been reached, as in both figures the saturation times are the same for all three mesons, regardless of the shape of each meson. In figure 1 (a) where $\varepsilon = 0.3$ GeV/fm^3, the equilibrium time for all meson species is around t = 22 fm/c and for figure 1 (b) at a higher energy density of ε = 0.4 GeV/fm^3, the equilibrium time is observed to have increased to t = 32 fm/c. These results show that an increase in energy density influences the particle multiplicity inside the periodic box, which affect the equilibration time.

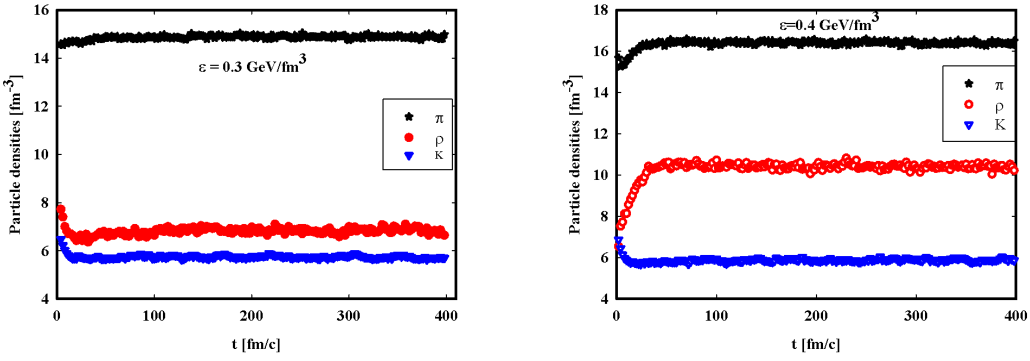


Figure 1: The time evolution of particle number densities of light meson species (π, ρ and K) at (a) $\varepsilon = 0.3$ GeV/fm^3 and (b) $\varepsilon = 0.4$ GeV/fm^3.

3.2. Thermal Equilibrium and Temperature

In this subsection the thermal equilibrium and the temperature from the energy distributions of different light meson species are studied. The possibility of the thermal equilibrium of the hadronic matter is studied by examining the energy distribution of the system in a box with periodic boundary conditions using the UrQMD model. The particle spectra are given by the momentum distribution as

$$\frac{dN_i}{d^3p} = \frac{dN}{4\pi EpdE} \propto Ce^{(-\beta E_i)}. \tag{3}$$

Figure 2 (a) and (b) represent the time evolutions of energy spectra of different meson species. The linear lines are fitted using the Boltzmann distribution, which is aproximated by $C\exp(-\beta E_i)$ from Eq. 3, where $\beta = 1/T$ is the slope parameter of the distribution and E_i is the energy of particle i. The results are plotted as a function of kinetic energy $K = E - m$, so that the horizontal axes for all the particle species coincide [9]. In figure 2 (a) and (b) it is observed that the slopes of the energy distribution converge to common values of temperatures at different times above t = 180 fm/c for ε = 0.2 GeV/fm^3 and above t = 250 fm/c for ε = 0.3 GeV/fm^3. In thermal equilibrium the system is characterized by unique temeperature T [9]. The thermal temperatures were extracted from the equilibrium state using the Boltzmann distribution such that T = 118.3 MeV for ε = 0.2 GeV/fm^3 and T = 150.1 MeV for ε = 0.3 GeV/fm^3.

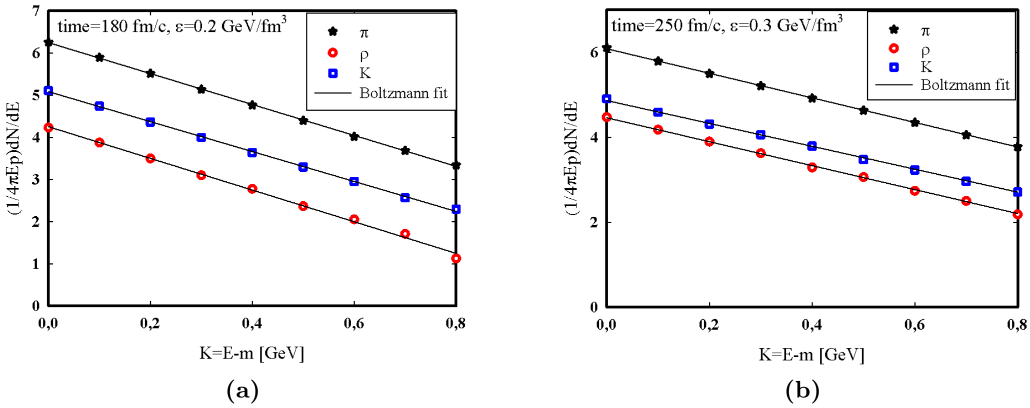


Figure 2: The energy distributions of light meson species (π, ρ and K) at (a) ε = 0.2 GeV/fm^3 and t = 180 fm/c and (b) ε = 0.3 GeV/fm^3 and t = 250 fm/c. The lines are the Boltzmann fit which gives the extracted temperatures of T = 118.3 MeV for (a) and T = 150.1 MeV for (b).

4. Thermal Conductivity Transport Coefficient

The transport coefficients, such as the thermal conductivity κ and the shear viscosity η, characterize the dynamics of the fluctuations of the dissipative fluxes in a medium [3]. The most often used method to investigate these coefficient is either through employing the kinetic theory or the field theory using the Green-Kubo formula [3].

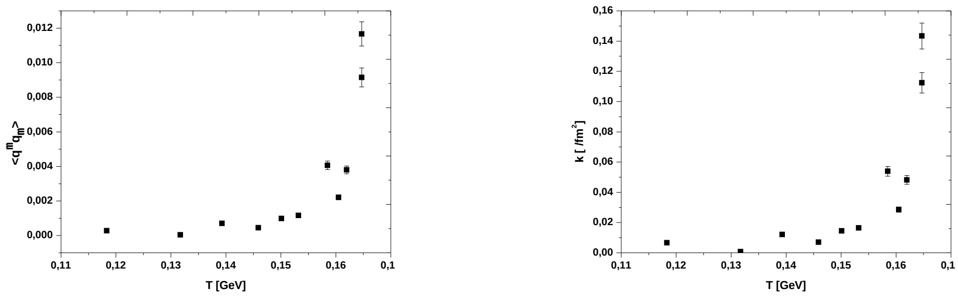
The knowledge of various transport coefficients is important for the dissipative fluid dynamical model. One can calculate the coefficient of thermal conductivity from the fluctuation-dissipation theorem theorem. The fluctuation-dissipation theorem tells us that the thermal conductivity is given by the heat current-current correlations [10]. Green and Kubo showed that the transport coefficients like heat conductivity, shear and bulk viscosity can be related to the correlation functions of the corresponding flux or the tensor in the thermal equilibrium [11]. The Green-Kubo formalism relates linear transport coefficients to near-equilibrium correlations of dissipative fluxes and treats dissipative fluxes as perturbations to local thermal equilibrium [12]. The relevant formular for the Green-Kubo relation for thermal conductivity can be written as [13]

$$\kappa = \frac{V}{3T^2} \int_0^\infty \langle \mathbf{q}_i\,(0)\,.\mathbf{q}_i\,(t)\rangle\, dt. \tag{4}$$

In Eq. (4) the brackets <...> stand for the equilibrium average, and no summation is implied over the repeated indices [3, 13]. κ is the thermal conductivity. The vector $\mathbf{q}_i$ is the Eckart's heat current along the $i = x, y$ and z axes which is defined as

$$\mathbf{q}^i = \frac{1}{V} \sum_{k=1}^{N} \mathbf{p}^i \left(\frac{\mathbf{p}^2}{\mathbf{p}_0^2} \right), \tag{5}$$

where $\mathbf{p}^i$ is the momentum along the $i = x, y$ and z axes, and $\mathbf{p}^2 = \mathbf{p}_0^2 - \mathbf{p}_x^2 - \mathbf{p}_y^2 - \mathbf{p}_z^2$, which can be extracted from the UrQMD model output file. If the evolution of the fluctuations of the fluxes is described by the Maxwell-Cattaneo equation [13]. We adopt a relativistic microscopic model, namely the UrQMD [8] and perform molecular-dynamics for a hadron gas of mesons in a box to compute the thermal conductivity coefficient of the hadron gas.



(a) **(b)**

Figure 3: (a) The square expectation value of the heat current and (b) the thermal conductivity of the hadronic gas as a function of temperature.

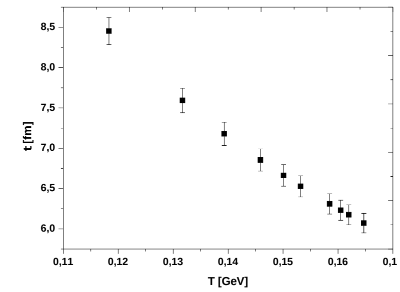


Figure 4: The relaxation time for the heat conductivity of a the hadronic gas as a function of temperature.

Figure 3 (a) shows the square expectation of the heat current results obtained from the UrQMD model. The heat current increases with increase in temperature. These results are in good comparison with those obtained in [10], where a different model named URASIMA was used. The UrQMD square expectation of heat current is much smaller than that obtained in [10]. The reason might be that for this study we considered a situation with only meson species and zero baryon number.

Figure 3 (b) shows the thermal conductivity κ of a hadronic gas, which increases with an increase in temperature. Saturation is reached below $T = 0.17$ GeV, where the hadronic gas with zero baryon number density is expected to be realized in the central high energy nuclear collisions [3]. According to our simulation, we observed a strong temperature dependence. The temperature behavior of the thermal conductvity is $\kappa \sim T^{2.88}$. The temperature dependence of thermal conductivity in this study is greater ($T^{2.88} > T^2$) than the one reported by [14], where the author used Effective Field Theory, and it is less ($T^{2.88} < T^5$) than the one reported by [10], where the author used a different simulation model called URASIMA and a different system which includes the baryon number densities.

Due to the smaller number of studies done on the thermal conductivity coefficient, it is difficult to make a proper conclusion from the results obtained, but from a comparison with the few related studies, one can agree that the results are in good comparison with those reported by [10]. At the moment it is not very clear where the large fluctuation around $T = 160$ MeV come from in the above figures. Thus a similar study will be done in the future which will include the baryon number density and different mesons species at higher energies and large number of events in order to check if one of these factors does play a role for this large fluctuation. Figure 4 shows the relaxation time for the heat flux of a hot hadronic gas as a function of the temperature calculated from the UrQMD model by fitting the heat correlation functions. The heat relaxation time decreases with an increase in temperature similarly to the one reported in [3, 10].

5. Conclusion

From the presented results, it can be concluded that it is possible to calculate thermal conductivity transport coefficient using the UrQMD model. More study is still required for a better understanding of the results and the coefficient. The future studies will focus on how the thermal conductivity transport coefficient is affected by adding different numbers of meson species in the box, including baryon number density, in order to compare with other studies such as that reported by [10, 15], as well as to compare to those who used different models and statistical approach [14, 16].

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