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Maxwell-Jüttner distributions in relativistic molecular dynamics

A. Aliano[a], L. Rondoni[b], and G.P. Morriss[c]

[1] Dipartimento di Fisica, Politecnico di Torino, Corso Duca degli Abruzzi 24, 1029 Torino, Italy
[2] Dipartimento di Matematica, Politecnico di Torino, Corso Duca degli Abruzzi 24, 1029 Torino, Italy
[3] School of Physics, UNSW, Sydney, Australia

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Abstract. In relativistic kinetic theory, which underlies relativistic hydrodynamics, the molecular chaos hypothesis stands at the basis of the equilibrium Maxwell-Jüttner probability distribution for the four-momentum p^α. We investigate the possibility of validating this hypothesis by means of microscopic relativistic dynamics. We do this by introducing a model of relativistic colliding particles, and studying its dynamics. We verify the validity of the molecular chaos hypothesis, and of the Maxwell-Jüttner distributions for our model. Two linear relations between temperature and average kinetic energy are obtained in classical and ultrarelativistic regimes.

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1 introduction

The study of relativistic fluids, both from the hydrodynamic and kinetic point of view has been widely investigated [1–5]. In this context, the relativistic Boltzmann equation

$$p^\nu \frac{\partial f}{\partial x^\nu} + m_0 \frac{\partial f F^\nu}{\partial p^\nu} = \int (f'_* f' - f_* f) \Omega \frac{d^3p'}{p'^0} \frac{d^3p_*}{p^0_*} \frac{d^3p'_*}{p'^0_*}, \quad (1)$$

represents the best known tool, which is based on a molecular chaos hypothesis, like the Boltzmann equation in classical kinetic theory. Here x^ν, p^ν, F^ν are respectively the position, momentum and force four-vectors, m_0 is the rest mass, Ω is the interaction cross-section, and f is the single particle distribution function. Collisionless relativistic plasmas are investigated by means of the relativistic Vlasov equation, obtained neglecting the collision term in equation (1). The equations of relativistic Hydrodynamics, which macroscopically describe relativistic fluids, are derived also from equation (1), similarly to the classical case.

The chaotic hypothesis, which underlies equation (1), explains how the microscopic components of a fluid reach a local equilibrium state. Classically, it is well established that this is a consequence of the interactions among the particles, as illustrated, for instance, by molecular dynamics [6].

In order to investigate the validity of the molecular chaos assumption in relativistic kinetic theory, we propose a simple model of N relativistic colliding particles, and investigate the properties of its dynamics.

In fact, to the best of our knowledge, many particle relativistic systems have only been studied either from a kinetic or hydrodynamic point of view, because the microscopic dynamics of such particle systems presents many difficulties. For instance, it is highly problematic to write covariant Hamiltonian (and the related 4-vector equations of motion) for the systems. Other difficulties concern: the choice of the reference frame, since every particle has a different proper time; the form of the interaction potential, since the action and reaction principle holds only for contact interactions; the effects of length contraction and time dilation. The consequence of this is that, as far as we know, no direct microscopic evidence for the molecular chaos hypothesis in relativistic dynamics has been provided.

To overcome this difficulty, we propose a non-covariant Hamiltonian written with respect to the center of mass frame, taken as the Lorentz rest frame, which yields the non-covariant equations of motion

$$\begin{cases} \dfrac{d\boldsymbol{x}_j}{dt} = \dfrac{c\,\boldsymbol{p}_j}{\sqrt{\boldsymbol{p}_j^2 + m_0^2 c^2}} \\ \dfrac{d\boldsymbol{p}_j}{dt} = \boldsymbol{F}_j^{WCA}(\boldsymbol{x}) \qquad j = 1, 2, ..., N, \end{cases} \quad (2)$$

[a] e-mail: antonio.aliano@polito.it
[b] e-mail: lamberto.rondoni@polito.it
[c] e-mail: G.Morriss@unsw.edu.au

where N is the number of particles. For the force $\boldsymbol{F}_j^{WCA}$ we propose to use

$$\boldsymbol{F}_j^{WCA} = -\sum_{i\neq j} \frac{\boldsymbol{r}_{ij}}{r_{ij}} \frac{\partial \Phi_{ij}^{WCA}}{\partial r_{ij}} = \begin{cases} \sum_{i\neq j} \frac{24\epsilon}{\sigma} \frac{\boldsymbol{r}_{ij}}{r_{ij}} \left[2\left(\frac{\sigma}{r_{ij}}\right)^{13} - \left(\frac{\sigma}{r_{ij}}\right)^{7} \right]; & r_{ij} < 2^{1/6}\sigma \\ 0; & r_{ij} \geq 2^{1/6}\sigma \end{cases} \tag{3}$$

where $\boldsymbol{r}_{ij} = (\boldsymbol{r}_i - \boldsymbol{r}_j)$, $r_{ij} = |\boldsymbol{r}_{ij}|$, Φ_{ij}^{WCA} is the Weeks-Chandler-Andersen interaction potential [7]; the quantities ϵ and σ are obtained from the Lennard-Jones (LJ) potential which defines Φ_{ij}^{WCA}, and represent respectively the depth of the LJ potential, and the distance at which it changes sign.

Therefore, particles move according to the relativistic dynamics when they do not interact, while their interactions are modelled classically, so that the total momentum and the total kinetic energy of particles are preserved by the collision process. Although this is not completely rigorous, our procedure meets all the microscopic requirements of relativistic kinetic theory, i.e. the invariance of the momentum 4-vectors.

In this paper we simulate a 2D system of N relativistic particles (with $N = 28$), through a MD algorithm, which implements the equations of motion (2, 3) with periodic boundary conditions, for a density $\rho = N/A = 0.2$ (with A the cell area), which is not a low density case. The simulations are performed for different initial kinetic energies corresponding to classical, relativistic and ultrarelativistic regimes. Furthermore, we take $\epsilon = \sigma = 1$.

In the low density limit, the contribution of the collisions is expected to become negligible, and the dynamics to tend to a fully covariant dynamics.

2 Results

Our results show that the simulated systems all reach an equilibrium state since their observables, such as the pressure, converge to an equilibrium value, while the probability distribution functions (PDFs) of the values of microscopic quantities like momentum p_x and kinetic energy ξ reach an invariant form. In particular, we find that the PDFs of p_x reduce to the Maxwell-Boltzmann (MB) distribution in the classical limit, as desired. This is due to chaos in the dynamics, which is evidenced by the fact that the numerically evaluated largest Lyapounov exponents are positive.

2.1 Probability distribution functions

The standard relativistic kinetic theory predicts that the PDF of p^α has the form of the Maxwell-Jüttner (MJ) distribution, $f_{MJ} = d\exp(-U^\alpha p_\alpha/k_BT)$, with d a normalization constant and U^α the hydrodynamic four-velocity (with $U^z = 0$) [1,2]. In the local rest frame, f_{MJ} can be written as

$$f_{MJ}(p_x, p_y) = d\,\exp\left(-a\sqrt{\frac{p_x^2+p_y^2}{m_0^2c^2}+1}\right), \tag{4}$$

where p_x, p_y are the spatial components of p_α, c is the speed of light, and where d and a are two constants related by the normalization condition

$$d = \left(\frac{1}{2\pi m_0^2c^2}\right)\frac{a^2e^a}{1+a}. \tag{5}$$

As well known [1,2], a involves the temperature of the system[1], because

$$a = m_0c^2/k_BT. \tag{6}$$

Integrating equation (4) over p_y, one obtains the PDF for p_x only:

$$g_{MJ}(p_x) = 2m_0cd\sqrt{\frac{p_x^2}{m_0^2c^2}+1}\;\; K_1\left(a\sqrt{\frac{p_x^2}{m_0^2c^2}+1}\right), \tag{7}$$

where $K_1(x)$ is the modified K-Bessel function of first order. Considering the kinetic energy $\xi = c\sqrt{\boldsymbol{p}^2+m_0^2c^2} - m_0c^2$, equation (4) can also be rewritten as

$$h_{MJ}(\xi) = \frac{2\pi}{c^2}d\,(\xi+m_0c^2)\exp\left(-a\frac{\xi+m_0c^2}{m_0c^2}\right). \tag{8}$$

It is interesting to observe that, if an expression like the MB distribution was written for the relativistic p_x, i.e. if one started from

$$f_{MB}(p_x,p_y) = f_{MB}(p_x)f_{MB}(p_y) = \frac{\tilde{a}}{\pi m_0^2c^2}\,\exp\left(-\tilde{a}\frac{p_x^2+p_y^2}{m_0^2c^2}\right), \tag{9}$$

the PDF of the relativistic kinetic energy ξ, after some calculations, would take the form

$$h_{MB}(\xi) = \frac{2\tilde{a}e^{\tilde{a}}}{m_0^2c^4}\,(\xi+m_0c^2)\,\exp\left(-\tilde{a}\frac{(\xi+m_0c^2)^2}{m_0^2c^4}\right). \tag{10}$$

Comparing equations (9, 10) with equations (7, 8), one notices that the MJ distribution is not merely the MB distribution with the relativistic p_x and ξ in place of the classical momentum and kinetic energy.

We fit the histograms constructed through our MD simulations to the PDFs given above, and for simplicity we take $m_0 = c = 1$.

The following figures 1, 2, 3 are obtained for different mean kinetic energies, where the mean kinetic energy is the time average of the total kinetic energy divided by the number of particles. The histograms are constructed

[1] By definition [8], classical is the regime with $a \gg 1$ and ultrarelativistic the regime with $a \ll 1$.

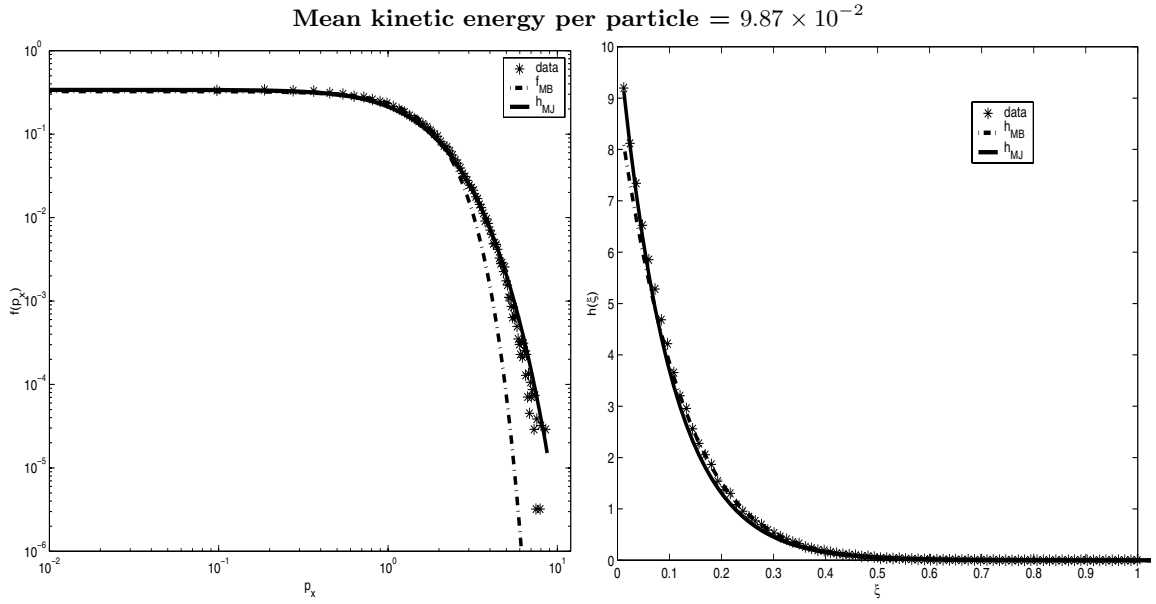

Fig. 1. Fit of the data for momentum p_x on a log scale (left panel). Fitted histograms of the kinetic energy ξ in linear scale (right panel). The parameter of the Maxwell-Jüttner PDFs takes the value $a = 10.4875$ for the PDF ofp_x yielding $k_BT = 0.095$ (left panel), and $a = 11.2595$ for the PDF of ξ leading to $k_BT = 0.089$ (right panel). The classical Maxwell Boltzmann PDFs fits well the data only in the low energy cases.

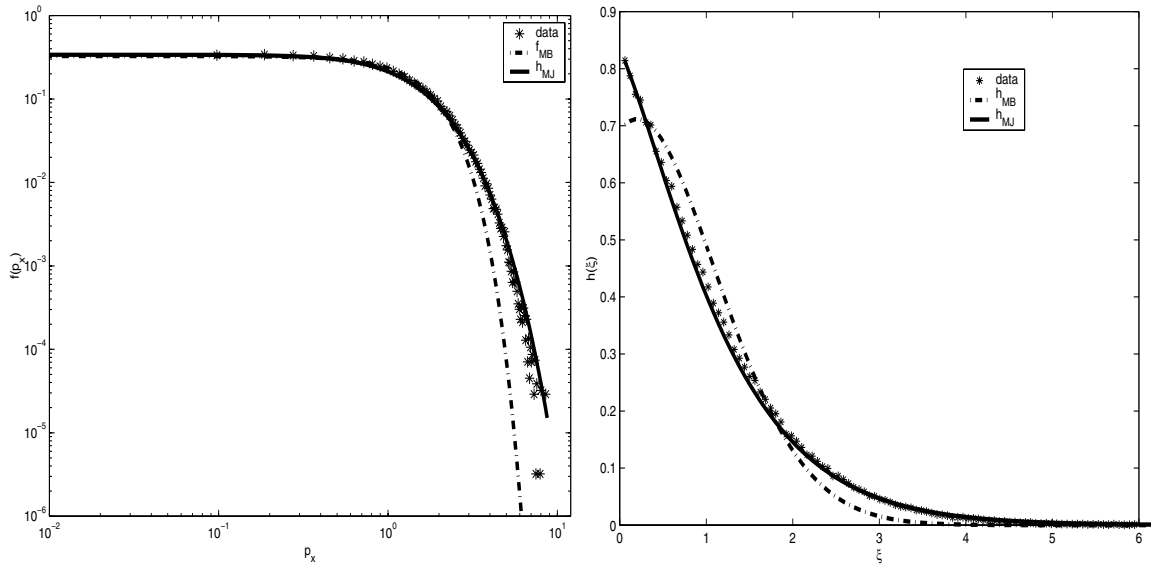

Fig. 2. Fit of the data for momentum p_x on a log scale (left panel). Fitted histograms of the kinetic energy ξ in linear scale (right panel). The parameter of the Maxwell-Jüttner PDFs takes the value $a = 1.4067$ for the PDF of p_x yielding $k_BT = 0.711$ (left panel), and $a = 1.4225$ for the PDF of ξ leading to $k_BT = 0.703$ (right panel). The classical MJ distributions fits better the data than the MB ones at these energies.

recording the instantaneous values of momentum p_x and kinetic energy ξ for a given particle. This operation is repeated every 200 timesteps, in order to decorrelate the recorded data.

For the Maxwell-Jüttner PDFs, if the parameters a and d are obtained as independent parameters by fitting the numerical data to equations (7, 8), the normalization condition (5) both for p_x and ξ is verified. This indicates that the MJ-PDF is indeed appropriate for our data, and that the data are consistent.

2.2 Measurement of temperature for a relativistic system

The microscopic definition of the temperature of a system composed by relativistic particles is an open is-

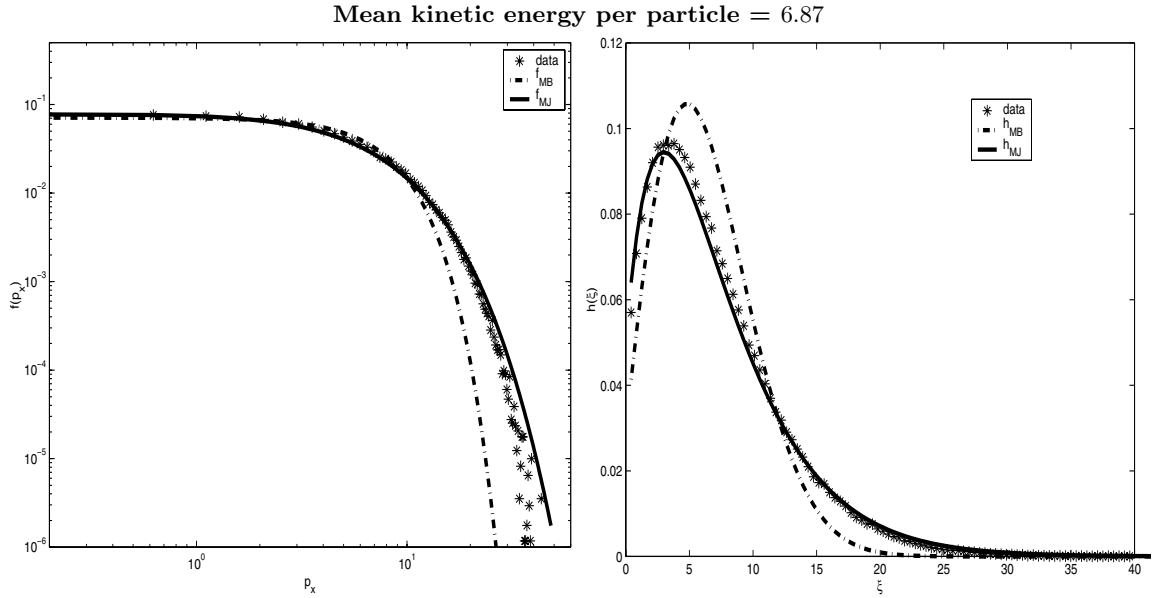

Fig. 3. Fit of the data for momentum p_x on a log scale (left panel). Fitted histograms of the kinetic energy ξ in linear scale (right panel). The parameter of the Maxwell-Jüttner PDFs takes the value $a = 0.2540$ for the PDF of p_x yielding $k_BT = 3.937$ (left panel), and $a = 0.2501$ for the PDF of ξ leading to $k_BT = 3.998$ (right panel). The MB does not fit the data at these ultrarelativistic energies.

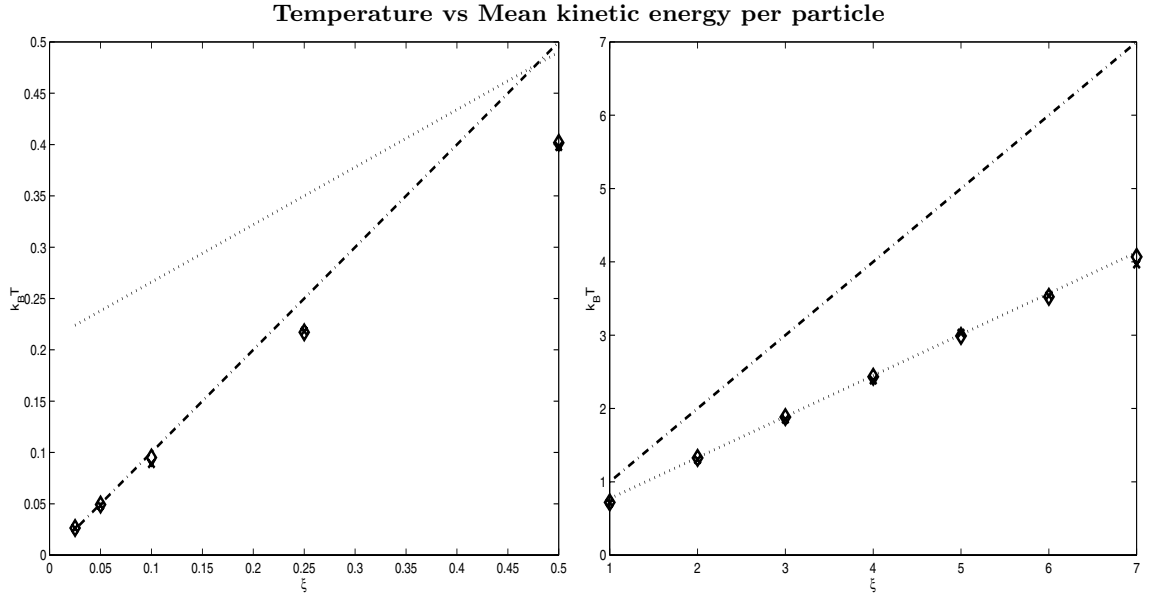

Fig. 4. Plot of temperature vs mean kinetic energy per particle. Temperatures are calculated through equation (6) from the fitting parameter $a^{-1} = k_BT$, obtained both for the kinetic energy($*$) and the p_x ($\diamond$). The two different calculations yield indistinguishable values in this figure. In the left panel the classical regime is plotted, while in the right one the ultrarelativistic limit is shown. In both panels the dotted lines represent the relation between k_BT and ξ valid in the low energy cases; the dash-dotted lines the relation between k_BT and ξ valid in the high energy cases.

sue [9]. However, the Maxwell-Jüttner PDF contains one parameter, which, in analogy with the classical Maxwell-Boltzmann PDF is identified with the quantity k_BT. Therefore, observing that the Maxwell-Jüttner PDFs fit well our histograms, it becomes reasonable to assume for our system $a^{-1} = k_BT$ as a definition of temperature obtained from the microscopic dynamics.

A linear relation between this temperature and the mean value of the kinetic energy per particle has been found for the classical and ultrarelativistic cases. For $k_BT = a^{-1} \lesssim 0.1$ (classical regime), the relation was found to be, as expected, $k_BT = \xi$, while for $k_BT = a^{-1} \gtrsim 1$ (relativistic and ultrarelativistic regimes), we verified a linear relation of the form $k_BT = 0.56\xi + 0.21$.

The transition between the two regimes takes place in a small range of kinetic energy values (cf. Fig. 4).

3 Conclusions

In this paper we have tested a 2D molecular dynamics model intended to simulate the microscopic dynamics of N relativistic colliding particles, with total constant energy E, and have observed its relaxation to an equilibrium state.

Our model satisfies the requirements of momentum and kinetic energy conservation before and after the collisions, underlying the equilibrium relativistic kinetic theory. The histograms found by these simulations for the momentum p_x, and for the kinetic energy ξ are well fitted by the PDFs of the standard relativistic kinetic theory, i.e. by the PDFs derived from the MJ distributions. In addition to this, the statistics of the dynamics of our model reduces to the classical one when the kinetic energy takes small values.

Our model suffers from the difficulties of not being fully relativistic, because the particle interactions are treated classically; therefore, it becomes more and more acceptable as the particle density decreases, or the collision rate tends to zero making the dynamics tend to a fully covariant form. Moreover, as we are going to report in [10], reducing densities does not produce any qualitatively different result, which indicates that in the limit of low collision rates the macroscopic behaviour of our systems is not substantially different from that of the higher density cases. This, together with the observed validity of the MJ distributions, provides a justification for our model, as a tool to simulate relativistic many particle systems. Otherwise, if this model is accepted, it affords a microscopic justification of the relativistic molecular chaos hypothesis, underlying relativistic kinetic theory and relativistic hydrodynamics.

Furthermore, linear relations of temperature and mean kinetic energy have been found both in classical and ultrarelativistic regimes. This allows us to obtain a definition of temperature in a relativistic system, something rather problematic in general [9], which deserves further investigations.

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