Freeze Out and the Boltzmann Transport Equation

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Abstract: Recently several works have appeared in the literature that addressed the problem of Freeze Out in energetic heavy ion reaction and aimed for a description based on the Boltzmann Transport Equation (BTE). In this paper we develop a dynamical Freeze-Out description, starting from the BTE, pointing out the basic limitations of the BTE approach, and the points where the BTE approach should be modified. 

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The Freeze Out (FO) is an important phase of dynamical processes. The connection of the kinetic description of this process and the Boltzmann Transport Equation (BTE) raised considerable attention recently. The phase-space (PS) distribution of post FO particles can be obtained from kinetic FO calculations. These were performed earlier in one-dimensional models, where the dynamics was governed by two constants: rethermalization and FO characteristic scales.

The FO is a kinetic process and one would think it can be handled perfectly by using the BTE, which may describe both equilibrium and non-equilibrium processes in a 4-dimensional space-time (ST) volume element like FO layer. This work and follows this approach. Our aim is to analyse the situation, discuss the applicability of BTE, and point out the physical causes, which limit the applicability of the BTE for describing FO.

FO is usually assumed to happen on sharp 3-dimensional ST hypersurfaces. However, the FO-fronts or FO-layers are not necessarily narrow, but they have a characteristic direction (or normal, dσμ), and it is more realistic to assume a continuous, 4-volume FO in a layer (or domain) of the ST. At the inside boundary of this layer there are only interacting particles, while at the outside boundary hypersurface all particles are frozen out and no interacting particles remain. Then the ST volume element, d4x, in the layer of interest can be converted into d4x → ds dσμ, where ds is the length element in the direction of the 4-vector dσμ (≡ dσμ for short), which can be time-like or space-like. Let us assume that the boundaries of this layer are approximately parallel, and thus thickness of the layer does not vary much.

The emission or FO probability may depend on physical processes, cross-sections, transition rates, and the actual PS distributions, f(x,p). Furthermore, f must be determined self-consistently during the FO, i.e. all conservation laws should be satisfied across this transition layer and overall entropy should not decrease!
duce a FO probability, which "feeds" the free component, $P_f \equiv P^{FO}(x, p)$, and the rest, $(1 - P_f)$, feeds the interacting one. Now, we can separate the two components into two equations. The sum of these two equations returns the complete BTE above:

$$p^\mu \partial_\mu f^f = \frac{1}{2} \int 12 D_4 f_1^i f_2^i P_f W_{12}^{p4}, \; (2)$$

$$p^\mu \partial_\mu f^i = -\frac{1}{2} \int 12 D_4 f_1^i f_2^i P_f W_{12}^{p4} + \frac{1}{2} \int 12 D_4 f_1^i f_2^i W_{12}^{p4} - \frac{1}{2} \int 2 D_4 f_1^i f_2^i W_{p2}^{p4}. \; (3)$$

The free component does not have a loss term, because particles in the free component cannot collide, and so, the free component cannot loose particles due to collisions. The first term of the second equation is a drain term, describing the escape or FO of particles from the interacting component. It is the inverse of the gain term for the interacting component. The last two terms are influencing the interacting component, and do not include the FO probability factors! Thus, these two terms drive the interacting component towards re-thermalization. For these the relaxation time approximation can be used.

$$p^\mu \partial_\mu f^i = -\frac{1}{2} \int 12 D_4 f_1^i f_2^i P_f W_{12}^{p4} + p_0 \frac{f^i_{eq} - f^i}{\tau_{rel}}. \; (4)$$

We see that the structure of the kinetic equations, used earlier, and the separation of the "escape" and "re-thermalization" terms come out in a simple straightforward way from the BTE.

However, the usual structure of the collision terms in the BTE is not adequate for describing rapid FO, in a layer which is comparable to the m.f.p. If we assume the existence of such a layer this immediately contradicts assumption (iii): the change is not negligible in the direction of $\dot{a}$. The assumption of "molecular chaos" is also violated in a FO process because number of collisions is not proportional with $f(x, p_1) \times f(x, p_2)$, but it is delocalized in the normal direction with $f(x_1, p_1) \times f(x_2, p_2)$. (The fact that the FO is a delocalized kinetic process, was already used in ref. 1 when integrals along the path of propagating particles were introduced, but the consequences regarding the details of the collision terms and the validity of the molecular chaos assumption were not discussed.)

Based on the above considerations, one might conclude that the changes of the distribution function are mediated by the transfer of particles, and consequently only slowly propagating changes are possible. If the FO layer propagates slowly, thus, its normal, $\dot{a}$, must always be space-like. This was a common misconception, where all "superluminous" shock, detonation, deflagration fronts or discontinuities were considered unphysical based on early studies 11. However, it was shown recently, that discontinuous changes may happen simultaneously in spatially neighbouring points, i.e. the normal of the discontinuity-hypersurface can be time-like 12.

This applies to the FO process also. Thus, the direction of characteristic or dominant change, $\dot{a}$, may be both space-like and time-like in the FO process.

From the all processes mentioned above (i.e. shocks, detonations, deflagrations etc.) the FO is the most special one, because the number of interacting particles is constantly decreasing as the FO proceeds, correspondingly the m.f.p. is increasing. In fact, it reaches infinity when the complete FO is finished. This means that we can not make the FO in finite layer of any thickness smooth enough to be modeled with the BTE. It is also obvious that if FO has some characteristic length scale, it is not proportional with the m.f.p. only, because the m.f.p. increases as the density of interacting component becomes smaller, while the FO becomes faster in this limit, so its characteristic scale should decrease.

To describe that the PS distributions change rapidly along the FO direction, we can introduce the Modified Boltzmann Transport Equation (MBTE):

$$p^\mu \partial_\mu f^f(x, p) = \frac{1}{2} \int 12 D_4 P_f W_{12}^{p4} f_1^i(x_1, p_1) f_2^i(x_2, p_2), \; (5)$$

$$p^\mu \partial_\mu f^i(x, p) = -\frac{1}{2} \int 12 D_4 P_f W_{12}^{p4} f_1^i(x_1, p_1) f_2^i(x_2, p_2) + p_0 \frac{f^i_{eq} - f^i}{\tau_{rel}}, \; (5)$$

where $x_k$ is the origin of colliding particles, i.e., the ST point where the colliding particles were colliding last, $x_k = x - u_k \tau_k$, $\tau_k$ is the collision time, $u_k^\mu = (\gamma_k, \gamma_k \vec{v}_k)$, $\gamma = 1/\sqrt{1 - \vec{v}^2}$ and $\vec{v}_k = \vec{p}_k/\gamma_k$. This is an essential modification if the PS distribution has a large gradient in the ST. This gradient defines a ST 4-vector, characterizing the direction of the process $\dot{a}$. In ref. 1 the direction $\dot{a}$ is also introduced, however, it is not discussed why and it is not connected to the delocalization of the BTE.

The symmetries and the assumption of local molecular chaos leads to the consequence that local conservation laws can be derived from the original BTE, i.e. $\partial_\mu T^\mu = 0$ and $\partial_\mu N^\mu = 0$ were $T$ and $N$ are given as momentum-integrals over the single particle PS distribution. After we delocalize the equations, this leads to new type of transport terms. The FO process results in additional particle and energy currents in the FO direction.

In the simplest case of infinitely narrow FO layer (FO hypersurface) between in and out domains the distribution function is given by $f = f_{in} \Theta_{in} + f_{out} \Theta_{out}$ and common BTE can be used everywhere except for the FO hypersurface. This case was actually studied without introducing MBTE in ref. 2 and the additional currents discussed above led to the possibility of the new type of Phase Transition - the so called three flux discontinuity, see 2 for more details.

The molecular chaos is also essential in the Boltzmann H-theorem. If we relax this condition, the solution of MBTE does not converge to a stationary thermal distribution, which enables us a simple thermo- and hydrodynamical treatment of the physical problem.
b. **Approximate Kinetic Freeze Out Models:** Let us present the schematic derivation of the kinetic FO model used by some of the authors earlier. This represents only one particular possibility and the general MBTE equation can be solved or approximated in other ways also.

If the ST distribution is non-uniform and the direction of steepest gradient can be clearly identified, one may replace one (or more) of the integrals over \( d^3p_1 \) (or \( d^3p_2 \)) by ST integrals over the origins of the incoming particle(s), \( d^3x' \), requiring that the particle reaches the ST point, \( x \), when needed. This requirement determines \( p_\mu \) for a given \( x' \). It is reasonable to assume that after converging some of the integrals to ST integrals and performing them, we get an effective FO term reflecting the properties of local PS distribution, transition rate, and ST configuration.

Let us execute two of the PS integrals for one incoming and one outgoing particle, \( f_2(x_1, p_1) = \frac{\mu f_{2}^i(x_1, p_1) W_{12}^{p_i}}{2} \). The result is then averaged over particles 2 and 4: \( W_{12}^{p_i} \). So, finally we obtain:

\[
p^\mu \partial_\mu f^i(x, p) = \frac{Q_2 V_4}{2} \int \frac{d^3p_1}{p_1^3} f_1^i(x_1, p_1) \mathcal{P}_f W_{12}^{p_i}, \tag{7}
\]

where \( Q_2 = \int \frac{d^3p_2}{p_2^3} \) and \( V_4 \) are invariant scalars.

Eq. (6) resembles eq. (3.27) in ref. [11], but one of the incoming particle distributions, \( f_2^i(x_2, p_2) \) is integrated out, and leads to an integral quantity, \( Q_2 \). This can be approximated by the invariant scalar density at \( \bar{x}_2 \), i.e., \( Q_2 \approx n_2(\bar{x}_2) \). Here \( V_4 \) is not given explicitly, but can in principle be calculated based on the distributions, \( f_1^i(x_1, p_1) \) and \( f_2^i(x_2, p_2) \), and the transition rate, \( W \). The resulting transition rate will then be averaged over particles 2 and 4: \( W_{12}^{p_i} \). Thus, we finally obtain:

\[
p^\mu \partial_\mu f^i(x, p) = \frac{Q_2 V_4}{2} \int \frac{d^3p_1}{p_1^3} f_1^i(x_1, p_1) \mathcal{P}_f W_{12}^{p_i}, \tag{7}
\]

where \( x_1 = (t_1, \bar{x}_1) = (t - \gamma_1 \tau_{\text{coll}}, \bar{x} - \bar{v}_1 \gamma_1 \tau_{\text{coll}}) = x - u_1 \tau_{\text{coll}}, \) \( \bar{v}_1 = \bar{p}_1/p_1^0 \) and \( u_1 = (\gamma_1, \bar{v}_1) \) indicates that the particle arrives at \( x \) starting earlier from another point \( x_1 \). As the first rough approximation we can take that \( \tau_{\text{coll}} \) is a mean collision time. The more general way to take into account particles coming from the different distances with corresponding probability factors is presented in [15]. In a rapid dynamical process the distributions at \( x \) and \( x_1 \) are not the same, as it was discussed above. Now, eq. (7) can be integrated either in the \( x_1 \)-space, or the \( p_1 \)-space.

In addition, the FO probability, \( \mathcal{P}_f \), may include integrated information about the FO process, e.g. the probability not-to-collide with anything on the way out. This should depend on the integral number of interacting particles on the way out.

For simplicity let us assume small angle scatterings, and the propagation of a single particle \( W_{12}^{p_i} \approx u_2^i \delta(p - p_1) \), then

\[
p^\mu \partial_\mu f^i(x, p) = \frac{Q_2 V_4}{2} f^i(x_1, p) \mathcal{P}_f u_2^i, \tag{8}
\]

where \( f^i(x_1, p) \) can be expressed in terms of \( f^i(x, p) \) and the 4-velocity, \( u^\mu \), of the particle with momentum \( \bar{p} \).
Let us now consider the FO situation, where we have a directed process in a layer. The dominant change happens in the direction of the normal of the FO hypersurface, \( d\sigma^\mu (d\sigma^\mu d\sigma_\mu = \pm 1) \) and it is negligible along the hypersurface of the front. This actually means that \( p^\nu \partial_\nu f(x,p) \approx (p^\nu d\sigma_\nu) \partial_\nu f(x,p) \). Inserting the above equation into (8) yields to a kinetic equation describing the directional derivative of the distribution function in the direction of the dominant change, \( d\sigma^\mu \), as

\[
d\sigma^\mu \partial_\mu f(x,p) = f^i(x_1,p) P^*_{esc} \quad (9)
\]

where \( f^i(x_1,p) \) reflects the system properties one m. f. p. earlier than the collision point and the escape probability \( P^*_{esc} = P_{esc}(x,p,f^i,d\sigma,w,P_f) \). The derivation above did neglect several details and features, however, reflects the basic structure of ad hoc kinetic FO models [3, 4, 5, 6].

c. Escape Probability: Here we just present briefly a direct estimate for the escape probability [12], detailed introduction and analysis of which will be given in [14].

The escape probability includes the collision rate and FO probability. The probability not-to-collide with anything on the way out, reasonably should depend on the number of interacting particles left in the way \( P_{esc} \), as

\[
P_{esc} = \frac{1}{N(x_1)} \left( \frac{L}{L - x^\mu d\sigma_\mu} \right)^a \cos(\Theta)^a \Theta(p^\mu d\sigma_\mu) \quad (10)
\]

where the power \( a \) is influencing the FO profile across the front, and the cut factor is eliminating negative contributions to FO. In papers [3, 4, 5, 6] authors used \( a = 1 \), and modeled FO in an infinite layer \( (L \to \infty) \), and a constant characteristic length \( \lambda \) were used instead of \( \lambda(x_1) \):

\[
P^*_{esc} = \Theta(p^\mu d\sigma_\mu) \frac{\cos(\Theta)}{\lambda} \quad (11)
\]

Comparing eqs. (10) and (11) one can see that we replaced the constant characteristic length \( \lambda \), which was clearly oversimplifying the situation, with \( \lambda'(x) = \lambda(x_1) \frac{1}{\langle n(x) \rangle} \), (for \( d\sigma^\mu = (0,1,0,0) \)) which contains two factors. The first is the collision rate, which is proportional with \( \frac{1}{\langle n(x) \rangle} \approx (n(x) \langle 1 \rangle) \), and this does not tend to zero even if we reach the outside boundary of the FO layer, as this parameter is characteristic to the interior region at \( x_1 \). The other is the generalized FO probability, which depends on the direction of the outgoing particle and on the number of interacting particles left in the way to collide with, i.e. \( \propto \frac{1}{\lambda}. \)

Now the new characteristic length \( \lambda'(x) \) gradually decreases as FO proceeds and the number of interacting particles decreases, and goes to 0, when the FO is finished, as it was discussed above.

The simple angular factor, \( \cos(\Theta) \), maximizes the FO probability of those particles, which propagate in the direction closest to the normal of the layer, \( d\sigma_\mu \). The quantities, \( \cos(\Theta) = p^\mu/|p| \) for FO in \( x \)-direction and \( \cos\Theta = 1 \) for FO in \( t \)-direction [4], are not Lorentz invariant. Therefore to make our description completely invariant we shall generalize it to \( P^*_{esc} = p^\mu d\sigma_\mu \approx \cos(\Theta) \).

So, we write the invariant escape probability, within the FO layer covering both the timelike and space-like parts of the layer [13], as

\[
P^*_{esc} = \frac{1}{\lambda(x_1)} \left( \frac{L}{L - x^\mu d\sigma_\mu} \right)^a \left( \frac{p^\mu d\sigma_\mu}{p^\mu u^\mu} \right)^a \Theta(p^\mu d\sigma_\mu) \quad (12)
\]

In refs. [4, 5, 6] the post FO distribution was evaluated for space-like gradual FO in a kinetic model with the escape probability [11]. The post FO distribution depends on the details of the escape probability and on the level of re-equilibration of the interacting component. Bugaev assumed earlier [7] that the post FO distribution is a (sharply) "Cut-Juttner" distribution, but the above mentioned model shows that this can only be obtained if re-equilibration is not taking place. The kinetic model provided an asymmetric but smooth PS distribution [4, 5], while the escape probability [12] yields a somewhat different, but also smooth PS distribution [13].

d. Conclusions: We have shown that the basic assumptions of BTE are not satisfied in the FO process, and so, the equation should be modified if used for the description of FO. We have also shown that earlier ad hoc kinetic models of the FO process can be obtained from our approach in a fully covariant way, and FO in space-like and time-like directions can be handled on the same covariant footing.
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