The impact of kinetic effects on the properties of relativistic electron–positron shocks

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Abstract
We assess the impact of non-thermally shock-accelerated particles on the magnetohydrodynamic (MHD) jump conditions of relativistic shocks. The adiabatic constant is calculated directly from first-principles particle-in-cell simulation data, enabling a semi-kinetic approach to improve the standard fluid model and allowing for an identification of the key parameters that define the shock structure. We find that the evolving upstream parameters have a stronger impact than the corrections due to non-thermal particles. We find that the decrease in the upstream bulk speed result in deviations from the standard MHD model up to 10%. Furthermore, we obtain a quantitative definition of the shock transition region from our analysis. For Weibel-mediated shocks the inclusion of a magnetic field in the MHD conservation equations is addressed for the first time.

1. Introduction
Shocks are common in the universe and a topic of high interest due to their importance in the acceleration of high-energy particles and the subsequent generation of radiation. The most prominent examples are the non-relativistic shocks in supernovae, which can provide an efficient acceleration of cosmic rays inside our galaxy [1], and relativistic shocks in gamma-ray bursts (GRB) [2]. A clear understanding of the shock properties and their connection to the structure of the fields and the distribution function of the particles is of critical importance to understand and to model many of the scenarios. In particular, as laboratory experiments start to explore in detail these conditions [3–6] and numerical simulations can capture many of the details of these structures [7–16], more detailed theoretical models are also required to explain and to predict the properties of relativistic shocks in different contexts [17–19].

The theoretical models to describe the shock properties are based on the hydrodynamic jump conditions, and assume a steady state, neglecting the involved kinetics. In particular, Blandford and McKee [20] considered strong shocks, which appear if either the upstream is cold and the energy per particle stays unchanged or if the upstream is ultra-relativistic, so that the rest mass energy can be neglected. In the latter case, energy and pressure are connected by the equation of state \(p = \epsilon/3\). However, due to the interaction with self-consistent fields in the shock, the particles can be trapped and accelerated in the shock, forming the characteristic high-energy tail in the distribution function, which has recently been reported in simulations (e.g. [11, 12]). The standard model of the hydrodynamic jump conditions assumes thermal spectra, neglecting the influence of accelerated particles. If the non-thermal tail is strong and the actual particle distribution deviates from such a spectrum, the pressure and energy densities in the downstream vary as well and lead to a modification of the steady-state conditions, which can be mathematically expressed by a modification of the adiabatic constant.

In this paper, we address the effect of such deviations and derive the jump conditions based on the actual particle distribution in the shock. In particular, we focus on the effects on the shock speed and the density compression ratio, which are the key parameters for determining the shock dynamics and energy transport. We start our analysis with a generalization of the theory for the shock jump conditions for an upstream population with non-zero temperature and discuss the impact...
of deviations from the idealized contributing parameters on the jump conditions. The theoretical predictions are then compared with fully self-consistent particle-in-cell (PIC) simulations. Our analysis demonstrates that the modification of the downstream adiabatic constant due to the development of the non-thermal tail as previously reported \[8, 11, 12\] can have a strong impact, but the decrease in the bulk Lorentz factor directly in front of the shock has the dominant influence on the jump conditions. Theory and simulations can be matched for a well-defined shock transition region, thus contributing to identify the different shock regimes.

The analysis is performed for a pure electron–positron plasma, as the expected effects on the adiabatic constant are qualitatively the same as for electron–ion plasmas if the plasma is initially unmagnetized. An initial magnetization suppresses the non-thermal acceleration in pure pair plasmas, and the role of ions then becomes important in this context \[21\].

2. Theoretical model

The starting point for the derivation of the shock jump conditions \[20\] is the conservation equations for mass, momentum and energy. We perform our calculations in the downstream rest frame in order to match the configuration of the simulations (see the next section). In the standard approach, the one-dimensional strong shock approximation, the upstream conditions \[20\] is the conservation equations for mass, momentum and energy. We perform our calculations in the rest frame \(\Gamma_1\), respectively. Thus, the conservation equations read

\[
\begin{align*}
n_1 u_{1i} &= n_2 u_{2i} \quad (1) \\
n_1 B_{1i} &= n_2 B_{2i} \quad (2) \\
\gamma_{1i} \rho_{1i} (1 + \sigma_i) &= \gamma_{2i} \rho_{2i} (1 + \sigma_2) \quad (3) \\
u_{1i} \mu_i (1 + \frac{\sigma_i}{2 \beta_{1i}^2}) + \frac{p_i}{n_1 u_{1i}} &= u_{2i} \mu_2 (1 + \frac{\sigma_2}{2 \beta_{2i}^2}) + \frac{p_2}{n_2 u_{2i}} \quad (4)
\end{align*}
\]

with \(u_{1i} = \gamma_i u_{1i}\), where \(\gamma_i\) denotes the Lorentz factor, \(\beta_{1i}\) is the transverse magnetic field, \(\beta_s\) is the magnetization, where \(\beta_s\) is the transverse magnetic field, \(n_i\) is the plasma density, and

\[
\mu_i = 1 + \frac{\Gamma_i - 1}{\Gamma_i} \frac{p_i}{\rho_i}
\]

is the specific enthalpy. The adiabatic constant \(\Gamma_i\) is defined by the relation between the energy density \(\epsilon_i\) and pressure density \(p_i = (\Gamma_i - 1)(\epsilon_i - \rho_i)\) with rest mass density \(\rho_i = n_i m c^2\).

We start our analysis by considering the case where the magnetic field contribution can be neglected, which is the standard approach for initially unmagnetized shocks \[10, 20\]. We will later discuss the influence of the self-generated magnetic fields on the jump conditions in the long time evolution of the shock. The shock speed can be determined by performing a Lorentz transformation in the downstream frame and combining equations (1)–(4), yielding

\[
\beta_{12} = \frac{(\Gamma_2 - 1)(\gamma_{12} \mu_1 - 1)}{\mu_1 \sqrt{\gamma_{12}^2 - 1}} \frac{\mu_1}{\gamma_{12}^2},
\]

which depends only on the upstream Lorentz factor \(\gamma_{12}\), the downstream adiabatic constant \(\Gamma_2\) and the upstream enthalpy \(\mu_1\). A non-zero upstream pressure \((\mu_1 > 1)\) increases the shock speed. This effect is weaker the higher the upstream Lorentz factor is and approaches the strong shock approximation for \(\mu_1 = 1\) \[9\]. The density ratio is given by

\[
\frac{n_2}{n_{12}} = 1 + \frac{\beta_{12}}{\beta_{12}} = 1 + \frac{(\gamma_{12}^2 - 1)\mu_1}{\gamma_{12}(\Gamma_2 - 1)(\gamma_{12} \mu_1 - 1)} \quad (6)
\]

and is decreased if the upstream pressure is taken into account. The deviations associated with non-thermal tails will have an impact on the adiabatic constant \(\Gamma_2\). In order to assess the influence of small deviations of the adiabatic constant \(\Gamma_2\) to the typically considered adiabatic constant of an ideal gas \(\Gamma_0^3\), we rewrite the adiabatic constant as \(\Gamma_2 = \Gamma_0^3 + \delta \Gamma_2\), where \(\delta \Gamma_2 \ll \Gamma_0^3\). The shock speed is now given by

\[
\beta_{12} = \beta_{12}^0 + \frac{(\gamma_{12} \mu_1 - 1)}{\mu_1 \sqrt{\gamma_{12}^2 - 1}} \delta \Gamma_2
\]

and, therefore, the correction of the adiabatic constant increases the shock speed by an amount of the order of \(\delta \Gamma_2\) for a highly relativistic upstream flow. The density ratio

\[
\frac{n_2}{n_{12}} \approx \frac{n_2^0}{n_{12}} = \frac{(\gamma_{12}^2 - 1)\mu_1}{\gamma_{12}(\Gamma_2^0 - 1)^2(\gamma_{12} \mu_1 - 1)} \delta \Gamma_2
\]

is decreased when the correction of the adiabatic constant is included. Typically, an adiabatic constant \(\Gamma_2^0 = 3/2\) for 2D, and 4/3 for 3D, is used to verify the jump conditions of relativistic shocks, e.g. \[12\]; therefore, the corrections to the density ratio are of the order of \(4 \delta \Gamma_2\) in 2D and \(9 \delta \Gamma_2\) in 3D for a relativistic upstream flow.

Deviations in the Lorentz factor of the flows can also affect the shock jump conditions. Following the previous approach, we define the Lorentz factor of the upstream flow as \(\gamma_{12} = \gamma_{12}^0 - \delta \gamma_{12}\), where \(\gamma_{12}^0\) is the initial Lorentz factor of the upstream flow and \(\delta \gamma_{12}\) its deviation. An increase in \(\delta \gamma_{12}\) reduces the shock speed and enhances the density ratio according to the Taylor expansion of the jump conditions (see appendix A).

The effects of the upstream pressure and of deviations of the adiabatic constant and upstream Lorentz factor on the density ratio are illustrated in figure 1, summarizing the previous findings and illustrating the stronger impact of the change in the upstream Lorentz factor.

3. Numerical simulations

In order to address the effect of the different parameters in realistic scenarios, where the shock structure evolves in time,
Figure 1. Effect of the upstream pressure, and of deviations of the adiabatic constant and upstream Lorentz factor on the density ratio. The increase in the upstream pressure and the slowing down of the flow increase the density ratio, whereas deviations in the adiabatic constant decrease the density ratio. All curves are plotted for $\gamma_1^2 = 20$. Black lines correspond to $\mu_1 = 1$, red lines to $\mu_1 = 2$, solid lines to $\Gamma_2 = 1.5$ and dashed lines to $\Gamma_2 = 1.52$.

in a self-consistent manner, we performed fully relativistic simulations of the shock formation and propagation with OSIRIS 2.0 [23, 24]. Using a fully kinetic model, the macroscopic quantities describing the shock structure can be calculated directly from the kinetic quantities and compared with our theoretical model. For a given distribution function $f(\gamma)$, the energy and pressure densities are calculated in the local rest frame of the fluid as

$$e := \frac{\tilde{e}}{nmc^2} = \int d^3p \frac{p^2}{\gamma} f(p)$$

and

$$p := \frac{\tilde{p}}{nmc^2} = \int d^3p \frac{p}{\gamma} f(p)$$

with $\gamma = \sqrt{1 + p^2}$. Note that the integrals reduce to double integrals for the 2D case. The adiabatic constant can then be calculated from the previously mentioned relation between energy and pressure densities as $\Gamma = 1 + p/(e - 1)$. For a relativistic Maxwellian $f(\gamma) = C \exp(-\gamma/\Delta \gamma)$ the adiabatic constant yields $\Gamma_{2D} = (2 + 3\Delta \gamma)/(1 + 2\Delta \gamma)$ for the 2D case and $\Gamma_{3D} = 1 + \Delta \gamma/[3\Delta \gamma - 1 + K_1(\Delta \gamma^{-1})/K_2(\Delta \gamma^{-1})]$ for a 3D geometry with $K_n(x)$ the modified Bessel functions of the second kind. The limiting values are $\Gamma_{2D} = 2$ for $\Delta \gamma \to 0$, $\Gamma_{2D} = 3/2$ for $\Delta \gamma \to \infty$ and $\Gamma_{3D} = 5/3$ for $\Delta \gamma \to 0$, $\Gamma_{3D} = 4/3$ for $\Delta \gamma \to \infty$.

We can immediately observe that, assuming a full thermalization of the upstream flow in the downstream, with a spread $\Delta \gamma = (\gamma_{12} - 1)/2$ [10], the density ratio equation (6) reduces to $n_{2}/n_{12} = 3$ in 2D, independent of the initial upstream Lorentz factor. Even for a highly relativistic flow, the deviations arising from the correction of the adiabatic constant can be noticeable, for instance $n_{2}/n_{12} = 3.1$ for $\gamma_{12} = 20$ and $n_{2}/n_{12} = 3.13$ for $\gamma_{12} = 15$ [8].

In reality, a more complex distribution function of the particles is expected due to the accelerated particle component.

Previous results found the best fit for a Maxwellian bulk plus a power-law tail:

$$f(\gamma) = \gamma^{-1} \frac{dn}{d\gamma} = C_1 \exp\left[-\gamma/\Delta \gamma\right]$$

$$+ C_2 \gamma^{-\alpha - 1} \min\left[1, \exp\left[-(\gamma - \gamma_{min})/\Delta \gamma_{min}\right]\right]$$

(11)

with $C_2 = 0$ for $\gamma < \gamma_{min}$ [10]. The contribution of this modified distribution to the macroscopic shock properties can now be addressed for the first time, using the self-consistent particle distribution from the simulations. The cumbersome analytical expressions for the energy and pressure densities are presented in appendix B. Large effects are expected for a very strong tail, which is given by a small $\gamma_{min}$ in combination with a small $\alpha$. In the case of relativistic shocks, these parameters are such that the contribution from the tail is weak.

In our simulations, the relativistic shock is created by injecting a charge neutral electron–positron beam with an isotropic thermal spread of $10^{-3}c$ and bulk Lorentz factor $\gamma_{12}^0 = 20$ along the negative $x_1$ direction. The particles are reflected at the opposite wall and interact with the incoming upstream particles, forming a shock. We use $10000 \times 300$ cells with a resolution $\Delta x = \Delta x_2 = 0.35c/\omega_p$, where $\omega_p = \sqrt{4\pi n_{12}^0 e^2/m_e}$ is the plasma frequency with $n_{12}^0$ the upstream electron density measured in the downstream frame at $t = 0$. The number of particles per cell is $3 \times 3$, the time step is $0.25 \omega_p^{-1}$, and the total simulation time is $4800 \omega_p^{-1}$.

The shock, which propagates along the positive $x_1$ direction, is formed after $t \approx 350 \omega_p^{-1}$. Figure 2 shows the important physical quantities at $t = 2395 \omega_p^{-1}$. The typical filamentary structure of Weibel-mediated shocks ahead of the shock front can be seen in the charge density as...
well as in the magnetic field (figures 2(a) and (d)) and the density compression factor is \( \approx 3 \) (figure 2(b)). The phase space diagram (figure 2(c)) shows the thermalized downstream region on the left hand-side and the shock transition region with escaped and reflected particles on the right-hand side of the shock front (located at around 1000 \( c/\omega_p \) for the conditions of figure 2).

At early times, the filamentary structure does not significantly affect the shock structure and its influence at later times is addressed in the following section. However, averaging over the transverse spatial component gives good qualitative agreement between the theoretical estimates and the simulation results throughout the entire shock propagation.

4. Discussion

The analysis of the density ratio associated with the shock front shows that this ratio can reach up to \( n_2/n_{12} = 3.2 \pm 0.08 \). This illustrates that when the shock structure is generated self-consistently the shock density ratio can deviate from the theoretical value \( n_0^2/n_{12} = 3 \), which is derived from the jump conditions for a cold plasma [20] and a Maxwellian distribution in the downstream with a thermal spread \( \Delta \gamma = 9.5 \) (leading to \( \Gamma_2 = 1.525 \)). We also observe a slight deviation from the shock velocity \( \beta_0 = 0.49 \) (\( \beta_{\text{measured}} = 0.48 \)). Since the impact on the density ratio is clearer, we will limit our detailed discussion to this quantity. In order to analyze the impact of the accelerated particles on the jump conditions we measured the adiabatic constant directly from the kinetic information of the particles in the simulation data as well as analytically from the fittings to the data in figure 3(a). For the analytical estimate we assume a particle distribution given by equation (11). Both methods provide essentially the same results. The adiabatic constant decreases logarithmically from initially \( \Gamma_2 = 1.5258 \) to \( \Gamma_2 = 1.5247 \) at the end of the simulation (figure 3(b)), which predicts a density change according to equation (A.4) of \( \delta n_2/n_{12} \approx 0.01 \) and does not explain by itself the density deviation which we observe in the simulations. We note that the changes in the adiabatic constant are very small and the fluctuations of the data points are almost on the same level as the total decrease in \( \Gamma \).

The particle distribution function in the downstream region is almost homogeneous along \( x_1 \) and varies slowly, whereas the physics in the shock transition region is highly dynamic. In the following, and in order to calculate the pressure and charge densities along the shock propagation direction, the particle distribution ahead of the shock is treated as a single bulk stream, which might not be appropriate for large simulation times, but in the early stages (up to \( t\omega_p \approx 2000 \)), the fraction of escaped or reflected particles is low compared with the bulk. The pressure density profile along \( x_1 \) is used to define the integration range for the quantities ahead of the shock, the Lorentz factor \( \gamma_{12} \) and the upstream enthalpy \( \mu_1 \). The peak in the pressure is considered as the transition between upstream and downstream regions and the integration range is varied up to 300 \( c/\omega_p \).
After the shock is formed, the Lorentz factor ahead of the shock deviates strongly from the initial value $\gamma_0 = 20$ (figure 4(a)), which leads to an increase in the density ratio according to figure 1. At the same time, the specific enthalpy has increased, which has a decreasing effect on the density ratio. Both quantities oscillate in phase, where a high enthalpy ratio significantly. On the other hand, the contribution of the decreasing upstream Lorentz factor is observed to have an important impact on the density ratio, and strongly depends on what is defined as the upstream region of the shock. The comparison of the results for different integration ranges shows that after an initial overshoot, the quasi-steady-state solution of the jump conditions for an integration range of $100 \omega_p$ converges with the data best. This suggests that only the vicinity of the shock front within this range significantly affects the shock properties.

Figure 6 compares the average downstream density from the simulations with different theoretical models listed in table 1. It is clear that the simulation results differ from the ideal model (M1—no changes in $\gamma_2$ and enthalpy). The inclusion of deviations from a Maxwellian distribution function of the downstream (M2) does not affect the density ratio significantly. On the other hand, the contribution of the decreasing upstream Lorentz factor is observed to have an important impact on the density ratio, and strongly depends on what is defined as the upstream region of the shock. The comparison of the results for different integration ranges shows that after an initial overshoot, the quasi-steady-state solution of the jump conditions for an integration range of $100 \omega_p$ (M5/M6) matches the data best. This suggests that only the vicinity of the shock front within this range significantly affects the shock properties.

If the contributions from the self-generated electromagnetic fields are considered, the resulting density ratio is slightly decreased. In equation (4), the first term on the left-hand side and the pressure term on the right-hand side are the dominant terms, and of the same order ($p_2/n_2 u_{2s} \approx u_{2s} \beta_{1s} = 20$). For the magnetization to become important, let us assume a contribution of 10%, so that it has to exceed $\sigma = 0.05$ as $\beta_{1s} \approx 1$. 

Figure 5. 2D plots: longitudinal and transverse currents in the shock region at times $t\omega_p = 500, 1000$. 1D plots: average $|E_1|$ (black), $|B_1|$ (green), $|E_2|$ (gray); $\gamma_2$ (red).
The total magnetization in our simulations is $\approx 0.05$ after a quasi-steady state has been reached, which makes it necessary to be included in the discussion of unmagnetized shocks. The additional decrease in the density ratio due to this contribution is of the order of 0.1, which is calculated from the conservation equations (1)–(4).

5. Conclusions

In conclusion, we have investigated the evolution of the shock properties when corrections from the usually considered fluid theory are taken into account due to the self-consistent evolution of shock properties, where kinetic effects are taken into account, and demonstrate that a quantitative comparison between shock parameters and simulations/observations should take into account deviations from the standard jump conditions.

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Appendix A. Changes in the jump conditions due to the Lorentz factor

The full expression of the shock speed is given by

$$\beta_{s2} = \frac{(\Gamma_2 - 1)(\gamma_{12}^0 \mu_1 - 1)}{\mu_1 \sqrt{\gamma_{12}^0} - 1}. \quad (A.1)$$

To obtain the influence of the upstream Lorentz factor $\gamma_{12} = \gamma_{12}^0 - \delta \gamma_{12}$, we do a Taylor expansion, yielding

$$\beta_{s2} = \beta_{s2}^0 \left(1 - \frac{(\Gamma_2 - 1)(\gamma_{12}^0 - \mu_1)}{\mu_1 (\gamma_{12}^0 - 1)^{3/2}} \delta \gamma_{12}\right). \quad (A.2)$$

From the density ratio

$$\frac{n_2}{n_{12}} = 1 + \frac{\beta_{s2}}{\beta_{s2}} = 1 + \left(\frac{\gamma_{12}^0 - 1}{\gamma_{12}^0 (\Gamma_2 - 1)(\gamma_{12}^0 \mu_1 - 1)}\right), \quad (A.3)$$

we obtain

$$\frac{n_2}{n_{12}} \approx \frac{n_2^0}{n_{12}^0} + \frac{\mu_1 (1 - 2 \mu_1)(\gamma_{12}^0 + (\gamma_{12}^0)^2)}{(\gamma_{12}^0)^2 (\Gamma_2 - 1)(\gamma_{12}^0 \mu_1 - 1) \delta \gamma_{12}}. \quad (A.4)$$

Appendix B. Analytical expressions for energy and pressure densities

For a distribution function consisting of a Maxwellian plus a power-law tail and an exponential cutoff, defined by equation (11), the analytical expressions for energy and pressure densities defined in equations (9) and (10) are given by

$$e = 2 \pi \left[C_1 \Delta \gamma (1 + 2 \Delta \gamma (1 + \Delta \gamma)) \exp (-\Delta \gamma^{-1}) + C_2 \times \left[\gamma_{\text{cut}}^{2-\alpha} - \frac{\gamma_{\text{cut}}^{2-\alpha}}{\alpha - 2} + \Delta \gamma_{\text{cut}}^{2-\alpha} \exp \left(\frac{\gamma_{\text{cut}}}{\Delta \gamma_{\text{cut}}} \right) \Gamma \left(2 - \alpha, \frac{\gamma_{\text{cut}}}{\Delta \gamma_{\text{cut}}} \right)\right]\right].$$
\[ p = \pi \left\{ 2C_1 \Delta \gamma^2 (1 + \Delta \gamma) \exp(-\Delta \gamma^{-1}) + C_2 \right\} \]
\[
\times \left[ \frac{\gamma_{\text{min}}^{2-\alpha} - \gamma_{\text{cut}}^{2-\alpha}}{\alpha - 2} - \frac{\gamma_{\text{min}}^{2-\alpha} - \gamma_{\text{cut}}^{2-\alpha}}{\alpha} + \Delta \gamma_{\text{cut}}^{-\alpha} \exp\left( \frac{\gamma_{\text{cut}}}{\Delta \gamma_{\text{cut}}} \right) \right] \frac{\Delta \gamma_{\text{cut}}^{\alpha - 1} - \alpha}{\Delta \gamma^\alpha \exp(-\Delta \gamma^{-1})} \]

with the exponential integral function \( E_\alpha(z) \).

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