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From the classical equations of motion to Relativistic Quantum Molecular Dynamics

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(arXiv:1210.3476 [hep-ph])

Outline

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Classical Dynamics

Let's begin simply. The classical dynamics for classical particles starts with the **Liouville equation**

$$\frac{\mathrm{d}A}{\mathrm{d}t}(\mathbf{q}, \mathbf{p}, t) = \frac{\partial A}{\partial t} + \frac{\partial A}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial A}{\partial \mathbf{p}}\frac{\partial \mathbf{p}}{\partial t}.$$

Knowing Hamilton's equations we can write a compact form.

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Knowing Hamilton's equations we can write a compact form.

Liouville equation

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\partial A}{\partial t} + \{A,\mathcal{H}\}$$

with $\begin{cases} \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}} \\ \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} \end{cases}$

Quantum Dynamics

The probabilistic aspect of particles can be considered by the **Wigner density** of a Gaussian wave function

$$f_W(\mathbf{q}_i, \mathbf{p}_i, t) \propto \exp\left(-\frac{(\mathbf{q}_i - \mathbf{q}_i^0(t))^2}{L}\right) \cdot \exp\left(-(\mathbf{p}_i - \mathbf{p}_i^0(t))^2 L\right)$$

Using the time dependent version of the **Ritz variational principle** we find

$$\frac{\mathrm{d}f_W}{\mathrm{d}t} = \{f_W, \mathcal{H}\}$$

(**Aichelin, Phys. Rep., 202:233 (1991)**)

Toward Relativistic Dynamics

To extend the classical dynamics to the relativistic one, let's try a simple example

$$\mathcal{H} = E = \sqrt{\mathbf{p}^2 + m^2 - V(\mathbf{q})}$$

From this Hamiltonian we find the well-known **equations of motion**

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \{\mathbf{q}, \mathcal{H}\} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}} = \frac{\mathbf{p}}{E}$$

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = \{\mathbf{p}, \mathcal{H}\} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} = \frac{1}{2E}\frac{\partial V}{\partial \mathbf{q}}$$

Toward Relativistic Dynamics

Then the problems are that :

- the energy E is not Lorentz invariant (energy conservation ?),
- we can't use an absolute time t (causality ?).

That is why people worked around these problems creating the **Quantum Field Theory**. Nevertheless it must be possible to formulate a relativistic dynamics to follow the **trajectories of particles**.

No Interaction Theorem

No Interaction Theorem : we cannot admit any interaction for a system with a speed close to the speed of light.

Assumptions :

- Invariant world-lines (respect of Poincaré's algebra),
- $8N$ independent degrees of freedom (q^μ, p^μ),
- Space-time dissociation (clusterization).

(**Currie, Rev. Mod. Phys. 35 (1963)**)

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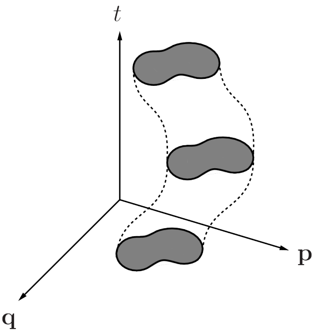
Equations of motion

Classical equations of motion

$$\frac{\partial \mathbf{q}_i}{\partial t} = \{\mathbf{q}_i, \mathcal{H}\} = \frac{\mathbf{p}_i}{E_i}$$

$$\frac{\partial \mathbf{p}_i}{\partial t} = \{\mathbf{p}_i, \mathcal{H}\} = \sum_k \frac{1}{2E_k} \frac{\partial V_k}{\partial \mathbf{q}_i} + \langle \text{ coll. } \rangle$$

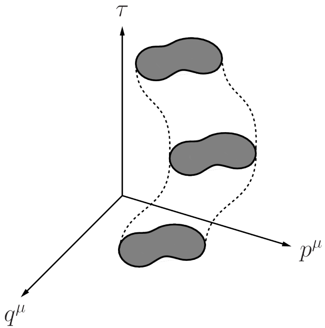


Classical dynamics is fine to describe particles with **low energy** in the **classical phase space** $(\mathbf{q}, \mathbf{p})$ but for relativistic particles we need to go to the **Minkowski phase space** (q^μ, p^μ).

Equations of motion

Relativistic equations of motion

$$\frac{\partial q_i^\mu}{\partial \tau} = \{q_i^\mu, \mathcal{Z}\} = 2\lambda_i p_i^\mu$$
$$\frac{\partial p_i^\mu}{\partial \tau} = \{p_i^\mu, \mathcal{Z}\} = \sum_k \lambda_k \frac{\partial V_k}{\partial q_i^\mu} + \langle \text{ coll. } \rangle$$



Here we have a new definition of equations of motion which are defined in a **constrained phase space** where λ plays the role of a factor which depends on the **reference frame**.

Relativistic Hamiltonian

$\mathcal{Z}$ is **not a classical Hamiltonian** !
It is just a **combination of the constraints**:

$$\mathcal{H} = E \quad \rightarrow \quad \mathcal{Z} = \sum_k \lambda_k \phi_k = 0$$

with relativistic factors λ_k, and constraints $\phi_k = 0$.
As well as $\mathcal{H}$, $\mathcal{Z}$ is a quantity related to a **time evolution parameter** : τ. In the classical case:

$$t = q_1^0 = q_2^0 = \dots$$

whereas in the relativistic case:

$$\tau = t \neq q_1^0 \neq q_2^0 \neq \dots$$

Constrained dynamics

We choose $2N$ constraints ϕ_k to **fix the times and the energies** of the N particles.

Relativistic constraints :

On-shell mass constraint for energy (conservation):

$$K_i = {p_i}^{\mu} {p_i}_{\mu} - {m_i}^2 + V_i = 0$$

and for the time fixation (causality):

$$\chi_i = \sum_{j \neq i} q_{ij}^{\mu} \; U_{\mu} = 0 \qquad \text{and} \qquad \chi_N = \frac{\sum_j q_j^{\mu}}{N} \; U_{\mu} - \tau = 0 \qquad U_{\mu} \overset{ref}{=} (1, \vec{0})$$

U_{μ} is the projector for the **reference frame** with time τ.

Constrained dynamics

We choose $2N$ constraints ϕ_k to **fix the times and the energies** of the N particles.

Relativistic constraints :

On-shell mass constraint for energy (conservation):

$$\frac{\partial E}{\partial \tau} = 0$$

and for the time fixation (causality):

$$\Delta q^0 = 0 \qquad \text{and} \qquad \langle q^0 \rangle - \tau = 0$$

U_μ is the projector for the **reference frame** with time τ.

Constrained dynamics

We still need the calculation of λ_k.
The **conservation of constraints** gives us :

$$\frac{\mathrm{d}\phi_i}{\mathrm{d}\tau} = \frac{\partial \phi_i}{\partial \tau} + \{\phi_i, \mathcal{Z}\} = 0$$
$$= \frac{\partial \phi_i}{\partial \tau} + \sum_{k}^{2N} \lambda_k C_{ik}^{-1} = 0.$$

with $C_{ik}^{-1} = \{\phi_i, \phi_k\}$ and finally :

$$\lambda_k = -C_{k2N} \frac{\partial \phi_N}{\partial \tau} = C_{k2N}.$$

A complex problem

We immediately see that λ_k are very important quantities, and therefore the constraints ϕ_k have to be chosen carefully. Indeed, we want to **avoid to invert** this matrix of constraints C_{ik}^{-1}.

Matrix of constraints

$$C_{ik}^{-1} = \{\phi_i, \phi_k\} = \begin{pmatrix} \{K_i, K_k\} & \{K_i, \chi_k\} \\ \{\chi_i, K_k\} & \{\chi_i, \chi_k\} \end{pmatrix}$$

We need some **additional conditions** on the constraints in order to find consistent equations of motion

A complex problem

$$\frac{\mathrm{d}q_i^\mu}{\mathrm{d}\tau} = \sum_{k=1}^{N} \lambda_k \frac{\partial K_k}{\partial p_{i\,\mu}} + \sum_{k=N+1}^{2N} \lambda_k \frac{\partial \chi_k}{\partial p_{i\,\mu}}$$

$$\frac{\mathrm{d}p_i^\mu}{\mathrm{d}\tau} = -\sum_{k=1}^{N} \lambda_k \frac{\partial K_k}{\partial q_{i\,\mu}} - \sum_{k=N+1}^{2N} \lambda_k \frac{\partial \chi_k}{\partial q_{i\,\mu}}$$

If $\{K_i, K_k\} \neq 0 \rightarrow \lambda_k \neq 0$ $(N+1 < k < 2N)$ and time constraints χ_k appear in the equations of motion.

Komar-Todorov condition

$$\{K_i, K_j\} = 2p_{ij}^\mu \frac{\partial V_i}{\partial q_j^\mu} + \{V_i, V_j\} \neq 0$$

(**Currie, Rev. Mod. Phys. 35 (1963)**)

Reference frame

Among all these constraints and conditions, there is an important concept to introduce: the choice of **reference frame**. From this choice depends:

- the **projector** $U_\mu \overset{ref}{=} (1, \vec{0})$, from which the time τ is correlated,
- and the **potential** V from the mass-shell constraint, from which the Komar-Todorov condition can be fulfilled (or not ...).

We can instinctively define two different frames:

- the **center of mass system** (cms) for 2 particles,
- and the **laboratory** (lab) where the full system is at rest ($\sum \vec{p} = \vec{0}$).

Reference frame

Consequently we define two different projectors:

$$u_{ij}^{\mu} = \frac{p_{ij}^{\mu}}{\sqrt{p_{ij}^{2}}} \stackrel{\text{cms}}{=} (1,0,0,0)$$

$$U^{\mu} = \frac{P^{\mu}}{\sqrt{P^{2}}} \stackrel{\text{lab}}{=} (1,0,0,0)$$

where $p_{ij}^{\mu} = p_i^{\mu} + p_j^{\mu}$ and $P^{\mu} = \sum_i p_i^{\mu}$. In the case of a system of 2 particles, these projectors are equal. We can use these projectors in the time constraint, and for the potential V in order to have an **invariant distance** (here for U^{μ}):

$$q_{T}{}_{ij}^{\mu} = q_{ij}^{\mu} - (q_{ij,\sigma} U^{\sigma}) U^{\mu}$$

Outline

Case of 2 particles

Using a potential $V = V(q_T)$, we find that the Komar-Todorov condition is fulfilled for the 2 particles case. Then

$$\frac{\partial q_i^\mu}{\partial \tau} = 2\lambda_i p_i^\mu$$
$$\frac{\partial p_i^\mu}{\partial \tau} = \sum_k \lambda_k \frac{\partial V_k}{\partial q_i^\mu}$$

with $\lambda_k = S_{kN}$ and $S_{ij}^{-1} = \{\chi_i, K_j\}$. Constraints are:

$$K_1 = {p_1}^2 - {m_1}^2 + V = 0$$
$$K_2 = {p_2}^2 - {m_2}^2 + V = 0$$

and

$$\chi_1 = q_{12}^\mu \; u_{12\mu} = 0$$
$$\chi_2 = \frac{1}{2}(q_1 + q_2)^\mu u_{12\mu} - \tau = 0$$

Case of 2 particles

Then we calculate the matrix of constraints:

$$S_{ij}^{-1} = \begin{pmatrix} 2\ p_1^\mu u_{12}^\mu & -2\ p_2^\mu u_{12\mu} \\ p_1^\mu u_{12}^\mu & p_2^\mu u_{12\mu} \end{pmatrix}$$

which we inverse:

$$S_{ij} = \begin{pmatrix} (4\ p_1^\mu u_{12\mu})^{-1} & (2\ p_1^\mu u_{12\mu})^{-1} \\ (4\ p_2^\mu u_{12\mu})^{-1} & (2\ p_2^\mu u_{12\mu})^{-1} \end{pmatrix}$$

and we find for 2 particles:

$$\lambda_1 = (2\ p_1^\mu u_{12\mu})^{-1} = \frac{1}{2E_1}$$

$$\lambda_2 = (2\ p_2^\mu u_{12\mu})^{-1} = \frac{1}{2E_2}$$

Case of 2 particles

The equations of motion become:

$$\frac{\partial q_i^\mu}{\partial \tau} = \frac{p_i^\mu}{E_i}$$

$$\frac{\partial p_i^\mu}{\partial \tau} = -\sum_{k=1}^{2} \frac{1}{2E_k} \frac{\partial V}{\partial q_{i_\mu}}$$

We use these equations in **6 dimensions**,
not in 8 because we have constrained proper times
and energies for each particle (4 equations).

Case of 3 particles

The case of 3 particles is the case of N. The third particle always acts on the 2 first particles as an **external field**.

Moreover for 3 particles, the Komar-Todorov condition can't be fulfilled. Both projectors give problems and we should work on a better definition of **relativistic potential**.

Nevertheless, assuming that the KT condition remains fulfilled, we can test the **effect of the projector** on the time constraint. For this example we simply take $V = 0$.

Case of 3 particles

We start with constraints for U^μ:

$$K_1 = {p_1}^2 - {m_1}^2 = 0$$
$$K_2 = {p_2}^2 - {m_2}^2 = 0$$
$$K_3 = {p_3}^2 - {m_3}^2 = 0$$

and

$$\chi_1 = (q_{12} + q_{13})^\mu U_\mu = 0$$
$$\chi_2 = (q_{21} + q_{23})^\mu U_\mu = 0$$
$$\chi_3 = (q_1 + q_2 + q_3)^\mu U_\mu / 3 - \tau = 0$$

Case of 3 particles

In this case the matrix of constraints is

$$S_{ij}^{-1} = \begin{pmatrix} 4\ p_1^\mu U_\mu & -2\ p_2^\mu U_\mu & -2\ p_3^\mu U_\mu \\ -2\ p_1^\mu U_\mu & 4\ p_2^\mu U_\mu & -2\ p_3^\mu U_\mu \\ 2/3\ p_1^\mu U_\mu & 2/3\ p_2^\mu U_\mu & 2/3\ p_3^\mu U_\mu \end{pmatrix}$$

and the inverse :

$$S_{ij} = \begin{pmatrix} (6\ p_1^\mu U_\mu)^{-1} & 0 & (2\ p_1^\mu U_\mu)^{-1} \\ 0 & (6\ p_2^\mu U_\mu)^{-1} & (2\ p_2^\mu U_\mu)^{-1} \\ -(6\ p_3^\mu U_\mu)^{-1} & -(6\ p_3^\mu U_\mu)^{-1} & (2\ p_3^\mu U_\mu)^{-1} \end{pmatrix}$$

As for the 2 particles case we find:

$$\lambda_k = \frac{1}{2E_k}$$

Case of 3 particles

If we take the other projector u_{ij}^{μ}:

$$\chi_1 = q_{12}^{\mu} u_{12\mu} + q_{13}^{\mu} u_{13\mu} = 0$$
$$\chi_2 = q_{21}^{\mu} u_{21\mu} + q_{23}^{\mu} u_{23\mu} = 0$$

and then :

$$S_{ij}^{-1} = \begin{pmatrix} 4\ p_1^{\mu}(u_{12} + u_{13})_{\mu} & -2\ p_2^{\mu} u_{12\mu} & -2\ p_3^{\mu} u_{13\mu} \\ -2\ p_1^{\mu} u_{12\mu} & 4\ p_2^{\mu}(u_{21} + u_{23})_{\mu} & -2\ p_3^{\mu} u_{23\mu} \\ 2/3\ p_1^{\mu} U_{\mu} & 2/3\ p_2^{\mu} U_{\mu} & 2/3\ p_3^{\mu} U_{\mu} \end{pmatrix}$$

whose inverse is highly non trivial.

Case of 3 particles

Finally if we keep the full system projector U^μ we find the same equations of motion than the 2 particles case, which is also the **same as “classical” relativistic equations**.

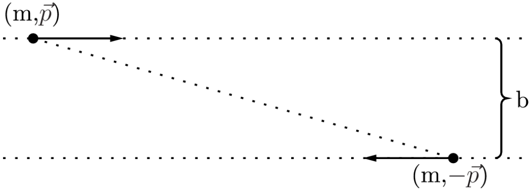
The other choice u^μ_{ij}, which was chosen in Sorge's paper for the RQMD code gives **unphysical trajectories** with velocities which can be above the speed of light.

(**Sorge, Ann. Phys. 192:266 (1989)**)

Outline

Time constraint test

We already know how the case of 2 particles is treated



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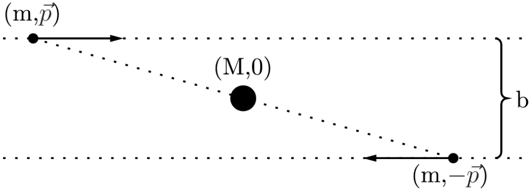

but what happens if we add an observing particle ?

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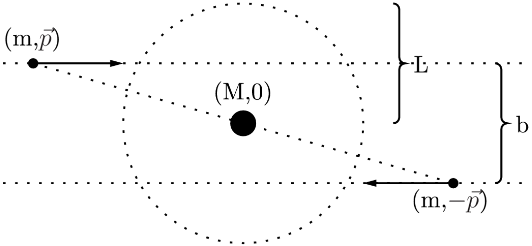
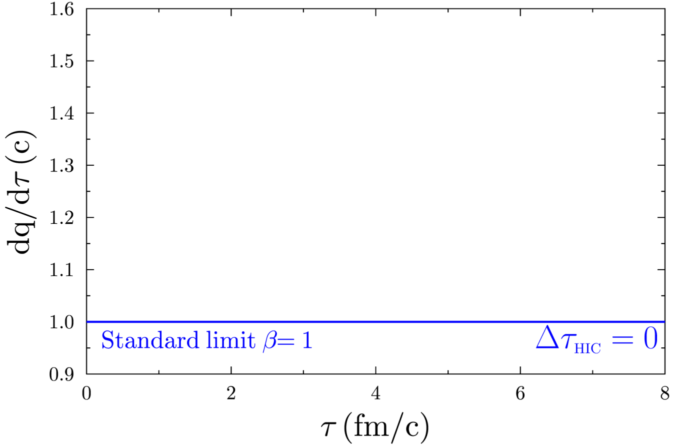


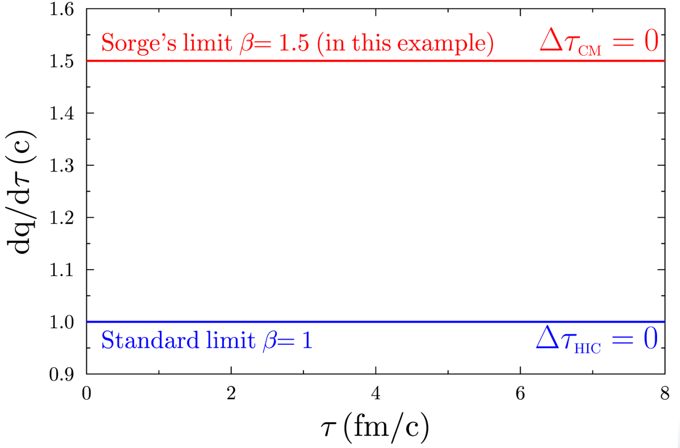
but what happens if we add an observing particle ?

$m = 10$ MeV, $\mathbf{p} = 1000$ MeV, $b = 0.1$ fm, $L = 1$ fm

Time constraint test



Time constraint test



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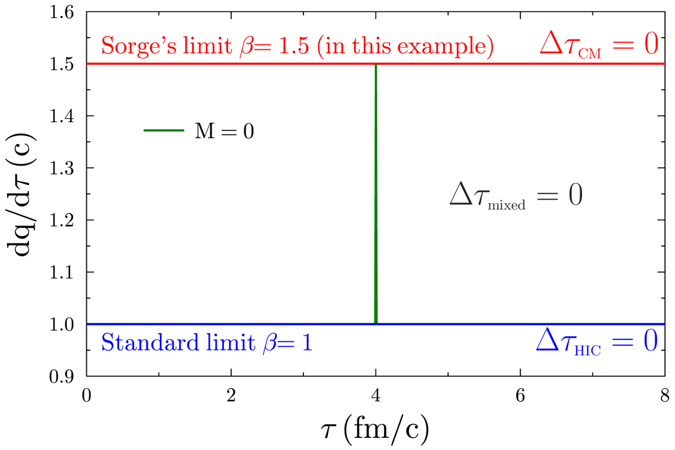

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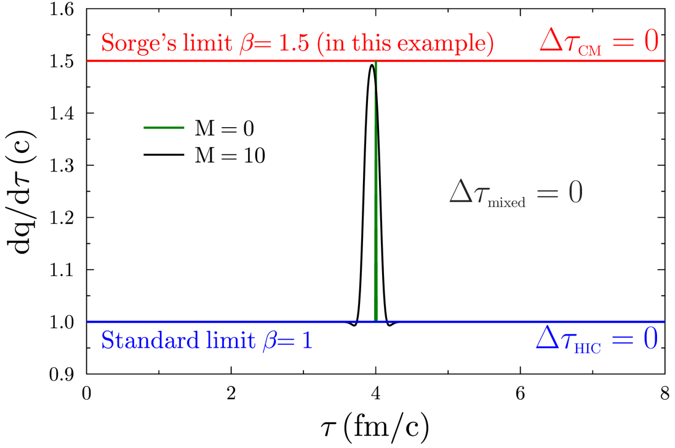

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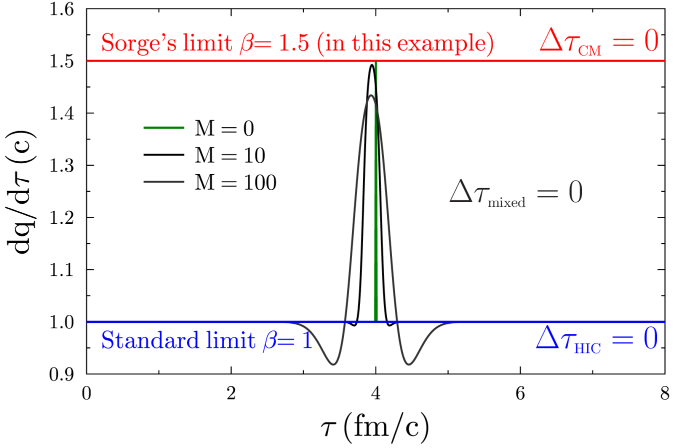

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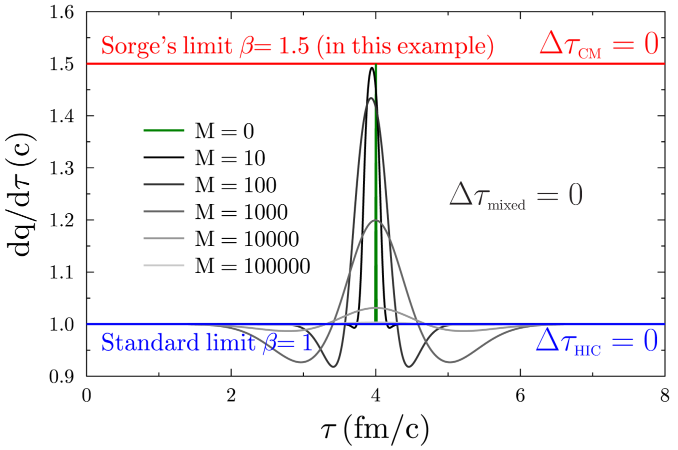
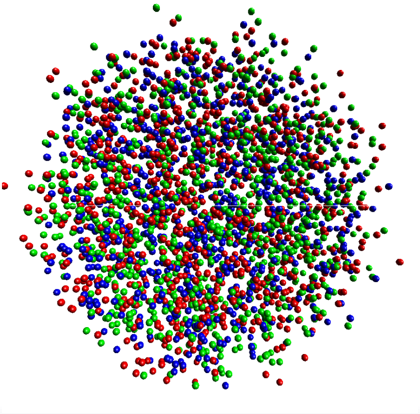
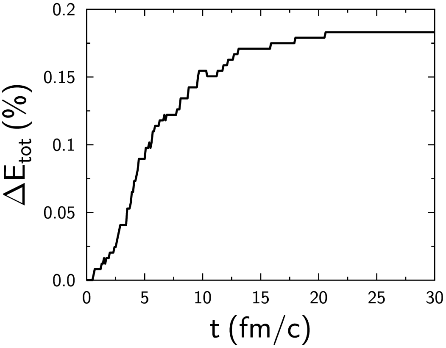


Heavy Ion Collision





Outline

Conclusion

What is the solution which works for relativistic dynamics ?

$$\frac{\mathrm{d}q_i^\mu}{\mathrm{d}\tau} = \frac{p_i^\mu}{E_i}$$
$$\frac{\mathrm{d}p_i^\mu}{\mathrm{d}\tau} = -\sum_{k=1}^{N} \frac{1}{2E_k} \frac{\partial V_k(q_T)}{\partial q_{i_\mu}} + \langle \text{coll.} \rangle$$

using the U^μ projector for $V(q_T)$. This is basically what is **already done** by all transport codes.

What do we still have to investigate ?

We must work on a **definition of relativistic potential** which fulfills the Komar-Todorov condition for few-body dynamics.

Thanks for your attention