Preliminary Results from the Parton-Hadron-Quantum-Molecular Dynamics (PHQMD) Transport Approach

J Aichelin$^{1,2}$, E Bratkovskaya$^{3,4}$, A Le Fèvre$^3$, V Kireyev$^5$ and Y Leifels$^4$

$^1$ SUBATECH, Université de Nantes, EMN, IN2P3/CNRS 4 rue Alfred Kastler, 44307 Nantes cedex 3, France
$^2$ Frankfurt Institute for Advanced Studies, Ruth Moufang Str. 1, 60438 Frankfurt, Germany
$^3$ GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstr. 1, 64291 Darmstadt, Germany
$^4$ Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany
$^5$ Joint Institute for Nuclear Research, Joliot-Curie 6, 141980 Dubna, Moscow region, Russia

Abstract. We present first results of the novel microscopic n-body dynamical transport approach PHQMD (Parton-Hadron-Quantum-Molecular-Dynamics) for the description of particle production and cluster formation (including hypernuclei) in heavy-ion reactions at relativistic energies. The PHQMD extends the established PHSD (Parton-Hadron-String-Dynamics) transport approach by introducing n-body quantum molecular dynamic type propagation of hadrons. This allows for a dynamical description of cluster formation based on the FRIGA (Fragment Recognition In General Application) model.

1. Introduction

After the discovery of a new state of matter, a plasma of quarks and gluons (QGP), in the experiments at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven and at the Large Hadron Collider (LHC) at CERN, the next goal is to study this new state at finite baryon density where some of the theories predict a first order phase transition [1, 2]. Two accelerators are presently under construction, the Facility for Antiproton and Ion Research (FAIR) in Darmstadt and the Nuclotron-based Ion Collider fAcility (NICA) in Dubna which will become operational in the next years. Moreover, presently running the Beam Energy Scan (BES) program at RHIC provides the experimental data at this energy regime, too. There scientific goal is to study those observables which may carry information on the existence of the plasma and especially of its phase transition in the hadronic world.

Fragment production at midrapidity is in general a very promising tool to study the phase space distribution of hadrons during the expansion. The multiplicity of the produced clusters is directed related to the phase space distribution of baryons at there creation point and therefore a change of the fluctuations like in the neighborhood of a first order phase transition will be directly reflected in the fragment multiplicity. In addition, without identifying fragments single particle observables cannot be correctly predicted. In 1.5 AGeV Au+Au collisions, the highest
energy where data on clusters formation are available presently, only 65% of the total baryon charge is observed as protons [3]. The rest is predominantly bound in small clusters which show a different rapidity distribution, a different flow and a different \( p_T \) spectrum. Therefore, even if one aims only at the investigation of single baryon spectra one has to identify fragments, otherwise a precise prediction is not possible.

The hypernuclei are one of the most promising probes to study the interaction between non-strange and strange baryons as well as the reaction dynamics of the heavy-ion collisions. The production of hypernuclei may shed light on our theoretical understanding of the dynamics of heavy-ion reactions which cannot be addressed by other probes. In particular, the formation of heavy projectile/target like hypernuclei elucidates the physics at the interface between spectator and projectile matter. Since the strange baryon comes necessarily from the overlap region the multiplicity as well as the rapidity distribution of the hypernuclei are related to the probability that strange baryons of a given rapidity are absorbed by the spectator matter by means of their potential interaction with the cold spectator matter. On the other hand, mid-rapidity hypernuclei test the phase space distribution of baryons in the expanding participant matter, especially whether strange and non strange baryons are in thermal equilibrium and whether their space time distribution is similar.

Here present preliminary resuls of the novel Parton-Hadron-Quantum-Molecular Dynamics (PHQMD) approach which allows to identify fragments is based on the collision integrals of the Parton-Hadron-String Dynamics (PHSD) approach [4, 5, 6, 7, 8] and the n-body potential interactions of QMD type models [11, 9, 10]. The original PHSD propagation in mean-field way (realized within the parallel ensemble method) is kept as an option, too, which will allow to investigate the differences in the both approaches.

The PHQMD includes the following features for the dynamical fragment identification: the final fragment yield can either be determined with a minimum spanning tree (MST) procedure [11] or with cluster finding algorithms based on the Simulated Annealing Clusterization Algorithm (SACA) [12].

i) The MST algorithm is based on spatial correlations and it is effective in finding the clusters at the end of the reaction. However, it is a rather simplified approach, which ignores the momentum correlations and energy balance in the found clusters.

ii) In order to identify the cluster formation at the early time of reactions, when the collisions between the nucleons are still going on and the nuclear density is high, the SACA method has to be used. The SACA finds this most bound configuration at any moment during the heavy-ion reaction with the help of the simulated annealing technique [12]. Combined with the QMD approach [11], SACA has been successfully used in the past to study spectra of fragments of a given charge by enclosing quantum shell effects, pairing as well as symmetry energy and hyperon nucleon interactions [14]. This possibility offers not only to study the physical origin of fragment formation but also clarifies experimental observations like bimodality [14, 15] or the large experimental inverse slope of the energy spectra which is about twice as large as the binding energy per nucleon of clusters [16].

2. The Parton-Hadron Quantum Molecular Dynamics (PHQMD) approach

The PHQMD approach unites the collision integrals of the PHS approach with the n-body interactions similar as in the Quantum Molecular Dynamics (QMD) approach.

2.1. Initialization

In the QMD approach the single-particle Wigner density of the the nucleon \( i \), \( f_i \), is given by (we use \( \hbar = c = 1 \))

\[
f_i(r, p, t) = \frac{1}{\pi^3 p^3} e^{-\frac{1}{2} (r - r_i(t))^2} e^{-\frac{1}{2} (p - p_i(t))^2}.
\]  

(1)
The total one-body Wigner density is the sum of the Wigner densities of all nucleons. To initialize the nucleons we choose randomly the position $r_i(t = 0)$ in a sphere with the radius $R = 1.14 A^{1/3}$. We take care that the distribution is smooth by requiring a minimal phase space distance between the nucleons.

Having placed the nucleons in coordinate space we calculate the expectation value of the potential energy, $< U(r_i, t) >$, of each nucleon $i$.

\begin{equation}
<U(r_i)> = \sum_j \int d^3r d^3r' d^3p d^3p' \ U_{ij}(r, r') f_i(r, p, t) f_j(r', p', t) \tag{2}
\end{equation}

with

\begin{equation}
U_{ij}(r, r') = U_{\text{Skyrme}} + U_{\text{Coul}} = \frac{1}{2} t_1 \delta(r - r') + \frac{1}{\gamma + 1} t_2 \delta(r - r') \rho^{\gamma - 1}(r) + \frac{1}{2} Z_i Z_j e^2 |r - r'|. \tag{3}
\end{equation}

Initially the expectation value of the potential energy $< U(r_i) >$ is negative. As the next step we chose then randomly the momenta $p_i(t = 0)$ with the requirement that the nucleons are bound

\begin{equation}
0 < \sqrt{m^2 + p_i^2(t = 0)} - m < - < U(r_i) >. \tag{4}
\end{equation}

where $m$ is the nucleon mass. This procedure gives a lower momentum to those nucleons which are located close to the surface because there the density is lower. Finally we take care that $\sum_i p_i(t = 0) = 0$ by adding a common momentum to all nucleons.

With so determined momenta and positions we calculate the average binding energy of the nucleons and compare the result with the Weizsacker mass formula. It turned out the we underestimate slightly the average binding energy independent of the size of the nucleus. To obtain the right binding energy we multiply finally all momenta by a common factor which is close to one and the same for all nuclei. It depends on the value of $L$.

Before the nuclei collide target and projectile are boosted into the nucleus nucleus center of mass frame and get Lorentz contracted.

### 2.2. Propagation

The propagation of the Wigner density is determined by a generalized Ritz variational principle \cite{11}, which has been developed for the Time Dependent Hartree Fock approach. Assuming that the width of the wave function is time independent and that the $n$-body Wigner density is the direct product of the single particle Wigner densities we obtain for the centroids of the Gaussian single particle wave functions:

\begin{equation}
\dot{r}_i = -\frac{\partial\langle H \rangle}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial\langle H \rangle}{\partial r_i}, \tag{5}
\end{equation}

where the expectation value of the total Hamiltonian is

\begin{equation}
\langle H \rangle = \langle T \rangle + \langle V \rangle = \sum_i \left( \sqrt{p_i^2 + m^2} - m \right) + \sum_i \sum_{j>i} \int dr dr' dp dp' \ f_i(r, p, t) V_{ij}(r, r', p, p') f_j(r', p', t). \tag{6}
\end{equation}
The potential consists of several terms:

\[
V_{ij}(\mathbf{r}, \mathbf{r}') = V_{\text{Skyrme}} + V_{\text{Coul}} = t_1 \delta(\mathbf{r} - \mathbf{r}') + t_2 \delta(\mathbf{r} - \mathbf{r}') \rho^{\gamma-1}(\mathbf{r}) + \frac{Z_i Z_j e^2}{|\mathbf{r} - \mathbf{r}'|}.
\]

\( (7) \)

The single-particle potential resulting from the convolution of the distribution functions \( f_i \) and \( f_j \) with the \( V_{\text{Skyrme}} \) interaction can be expressed as

\[
<U_{i \text{Skyrme}}(\mathbf{r}_i, t) > = \alpha \left( \frac{\rho_{int}(\mathbf{r}_i, t)}{\rho_0} \right) + \beta \left( \frac{\rho_{int}(\mathbf{r}_i, t)}{\rho_0} \right)^\gamma,
\]

\( (8) \)

where \( \rho_{int} \) is the interaction density obtained by convoluting the distribution function of a particle with the distribution functions of all other particles of the surrounding medium.

\[
\rho_{int}(\mathbf{r}_i, t) = C \sum_{j \neq i} \left( \frac{4}{\pi L} \right)^{3/2} e^{-\frac{4}{L}(\mathbf{r}_i(t) - \mathbf{r}_j(t))^2}
\]

\( (9) \)

C is a constant which has to be adjusted to reproduce the density profile of the nuclei.

The nuclear equation of state (EoS) describes the variation of the energy \( E(T = 0, \rho/\rho_0) \) when changing the nuclear density in infinite matter to values different from the saturation density \( \rho_0 \) for zero temperature. In infinite matter the density is position independent and we can use eq. (8) to connect our Hamiltonian with nuclear matter properties because for a given value of \( \gamma \) the parameters \( t_1, t_2 \) in eq. (7) are uniquely related to the coefficients \( \alpha, \beta \) of the EoS, eq. (8). Values of these parameters for the different model choices can be found in Tab. 1.

|   | \( \alpha \) (MeV) | \( \beta \) (MeV) | \( \gamma \) |
|---|-------------------|------------------|------|
| S | -390              | 320              | 1.14 |
| H | -130              | 59               | 2.09 |

\( \text{Table 1. Parameter sets for the nuclear equation of state used in the QMD model} \)

3. Results

QMD type approaches have been very successfully in the past to describe many details of the fragment formation at energies below \( E_{kin} = 200\ A\text{MeV} \) \([17, 14, 16, 17, 18]\). They could reproduce charge yields, fragment multiplicities, fragment spectra and complex phenomena like bimodality. At these energies the fragmentation of spectator matter is the dominate mechanism and cluster identifications methods like the minimum spanning tree method or the SACA method \([19]\) could identify the produced cluster.

The MST method identifies cluster at the end of the reaction when nucleons and fragments are well separated in phase space. In MST two nucleons are considered as part of a cluster if their distance is smaller than \( r_{min} < 3\ fm \). Additional momentum cuts do not change the result because unbound nucleons have separated at this late time to a distance larger than \( r_{min} \). The drawback of the MST method is that it can identify fragments only at the end of the reaction and therefore it can not be used to study how fragments are formed during the reaction.

To overcome this limitation we have developed the Simulated Annealing Cluster Algorithm (SACA) approach \([19]\). It is based on the idea of Dorso and Randrup \([13]\) that the most bound configuration of nucleons and fragments during the reaction has a large overlap with the final
distribution of fragments and free nucleons. Dorso and Randrup could demonstrate this for small systems and Puri and al. [19] found out that it is also true for large systems. To obtain the most bound configuration during the reaction one applies a simulated annealing algorithm. In this algorithm in each iteration step one identifies one nucleon. If this nucleon is bound it can become unbound or can become part of another cluster. If it is unbound it can become part of a fragment. After each iteration step one calculates the total binding energy of the system neglecting the interaction among nucleons which belong to different fragments. If the new configuration is more bound it is kept, if it is less bound it is kept with a given probability to avoid that the procedure ends in a local and not in a global minimum. The binding energy is calculated with the same interaction which is also used for the time evolution of the nucleons (eq. (3)). For details we refer to [19].

The PHQMD proton rapidity distribution for central AuAu collisions at beam energies at 1.5 AGeV is shown in Fig. 1 and compared with the experimental result of the FOPI collaboration [20]. We display as well the distribution of all charges. First of all we see that the stopping in this reaction is quit nicely reproduced giving the right rapidity distribution. Second we see that quite a number of all charges are bound in clusters. PHQMD overpredict even the number of bound nucleons at midrapidity resulting in an underestimation of the height of the experimental proton rapidity distribution. Next we investigate the results of

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig1}
\caption{Scaled experimental rapidity distribution, $y_0 = y/y_{cm}$, of free protons observed in central AuAu reactions at 1.5 AGeV [20] in comparison with the PHQMD results. The red line shows the rapidity distribution of all bound and unbound protons whereas the black line indicates those protons which are considered as free after the fragments have been determined by MST.}
\end{figure}

the ALADIN collaboration which has measured the fragment formation at beam energies of around 800 AMeV [21]. This is presently the highest energy for which data on heavy fragments are available. For this investigation we use a hard equation of state. One of the key result of the Aladin collaboration was the "rise and fall" of the multiplicity of intermediate mass fragments $3 \leq Z \leq 30$ emitted in forward direction. Plotting this multiplicity as a function of the sum of all forward emitted bound charges, $\sum_i Z_i \Theta(Z_i - (1 + \epsilon))$ one obtains a curve which is for Au projectiles independent of the beam energy in the intervall $600 \ AMeV \leq E_{beam} \leq 1000 \ AMeV$ and also independent of the target size. Up to now this "rise and fall" has not been described by transport approaches. In Fig. 2 we display our results in comparison with the minimum bias ALADIN data. We see clearly the rise of the multiplicity of intermediate mass fragments for small values of $Z_{\text{bound}}$ independent of the identification of fragments which we use. The multiplicity is also correctly reproduced for large $Z_{\text{bound}}$ if we apply the SACA algorithm but
Figure 2. Rise and all of the multiplicity of intermediate mass fragments as a function of the total bound charge. Both quantities are measured for forward emitted fragments. We compare the results of PHQMD for different approaches to identify fragments with the experimental data [21].

MST underestimates there the multiplicity. This is due to the fact that in MST in the average one of the intermediate mass fragments which is identified by SACA is considered in MST as part of the largest fragment. We can conclude that PHQMD reproduces one of the most complex fragment data in this energy domain.

It is interesting to see what our present fragment algorithm gives if we increase the beam energy. In Fig.3 we display the rapidity distribution of fragments for central AuAu collisions at $E_{beam} = 3.5 \text{ AGeV}$. The fragments are identified with the MST algorithm. We display this distribution for two times 30fm/c and 90 fm/c and for $Z=2$ fragments as well as for hyper-nuclei, i.e. $\Lambda$ and $\Sigma_0$ which form a cluster with at least one other nucleon. Besides in the target and projectile rapidity region where fragment formation and interactions still continue because the nucleons are close not only in momentum but also in coordinate space the fragment distribution changes little between 30 and 90 fm/c. This confirms that - in contradistinction to the coalescence model - in PHQMD the fragment yield is time independent and that the fragments are formed dynamically. We see as well an appreciable number of $Z=2$ fragments and hyper-nuclei. Even if the MST method does not allow for a quantitative description of the yield our calculation shows the potential of the future experiments of the BM@N detector at Dubna to study the formation of light hyper-nuclei.

4. Conclusion
We have presented preliminary results of a new transport model, PHQMD, to study the dynamics of heavy ion collisions at beam energies between 500 AMeV and the highest LHC energies. It extends the studies with the QMD model at lower beam energies. This model includes the collision dynamics as well as the partonic interaction from the PHSD approach. It extends the PHSD approach by replacing the one body mean field dynamics by a n-body quantum molecular dynamics which propagates all correlations and fluctuations and which is therefore a basis to study the fragment formation in heavy ion reactions.

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Figure 3. Rapidity distribution of bound and unbound protons, of Z=2 fragments and of hyper-nuclei for central AuAu collisions at $\sqrt{s} = 200$ AGeV.

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