Deuteron and entropy production in relativistic heavy ion collisions

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Employing an extended version of the Boltzmann-Uehling-Uhlenbeck equation, we present simulations of the reaction 800 MeV/nucleon Ca + Ca. Deuteron spectra are calculated from the model without *ad hoc* assumptions. Absolute values of the proton and deuteron spectra are in good agreement with experiment. The dependence of the total deuteron yield on the nuclear equation of state is investigated and found to be weak. Both entropy and freeze-out density are strongly dependent on impact parameter. This suggests, in particular, that the freeze-out density has no physical meaning. Methods for calculating entropy are discussed and numerically compared.

I. INTRODUCTION

Several years ago, Siemens and Kapusta[1] argued that the entropy generated in high energy heavy ion collisions could be inferred from the final state production ratio of deuterons to protons. Since then, the mechanism of cluster production and its relation to entropy production have been subjects of a lively and still unsettled debate. In this paper we report on a study of deuteron production, entropy production, and their relation, using as a dynamical model an extended version of the recently introduced[8,9] Boltzmann-Uehling-Uehlenbeck (BUU) equation applied to the 800 MeV/nucleon Ca + Ca reaction.

The salient feature of the deuteron momentum distribution, its approximate proportionality to the nucleon distribution squared, unfortunately carries little physical information. This follows directly from the fact that it is hard to imagine any reasonable theory in which nucleons coalesce when their relative momentum lies much outside the range defined the deuteron wave function. Thus a large variety of physically very different theoretical approximations (thermodynamics,[2] coalescence,[3] sudden approximation[4]) have all agreed on this one feature.

The simplest nontrivial feature of cluster production which theory must explain is the constant in the aforementioned proportionality, and its dependence on various collision parameters. A general formalism capable of doing this was introduced some time ago.[5] Since it simply consists of a reformulation of ordinary scattering theory in terms of the density operator, it is not a dynamical theory *per se,* and consequently requires, in addition to itself, some model of the density operator describing the reaction to produce theoretical cross sections. (Currently available dynamical models are generally unable by themselves to describe cluster formation.) This formalism can be adapted to any dynamical model (fluid dynamics, intranuclear cascade, etc.) Until recently, however, few such models could be computed in sufficient detail to use this approach.

An application of this scattering theory approach specialized to the intranuclear cascade model (INC) of the time-dependent density operator was presented in Ref. 6. Its results were of course dependent on (and a test of) the validity of the underlying INC model. An important shortcoming of the INC model is its lack of coherent scattering, which can be represented approximately by the presence of a nuclear mean field. This distorts its distributions in kinematic regions where large numbers of nucleons tend to move off as a group, namely, at low velocities in the nucleon-nucleon, target, and projectile center of mass frames. Since many reaction products emerge at these velocities, they contribute significantly to the entropy. Thus lack of a mean field is a deficiency of the INC model considered as a tool to calculate entropy. This problem has been largely eliminated in the BUU model which contains both a self-consistent mean field and corrections due to Pauli blocking.

Another shortcoming in the calculation in Ref. 6 stemmed from limitations on computing time. The complete expression for deuteron production consists of a sum of contributions from each neutron-proton pair in the system. For each pair one must evaluate an alternating series which can be heuristically interpreted as describing the pair's creation and destruction as deuteronlike correlations ("primordial deuterons") during the course of the reaction. It was shown that for large enough momenta deuterons, the last (positive) term dominates the series since the others tend to cancel by pairs. This approximation (the "generalized coalescence model") greatly reduces one's computational effort. Its use, however, limited the results of Ref. 6 to large momentum deuterons. A complete calculation of all the terms in the series is presented here.

Another approach to these questions was advanced by Bertsch and Cugnon.[7] They calculated the Boltzmann entropy of a heavy ion system from the phase space distribution generated again by an INC model and compared it to that obtained in Ref. 1. In addition to being subject to the limitations of the INC model, use of the Boltzmann entropy precluded taking into account the effect of correlations on the value of the entropy. Cugnon[16] has also explored the impact parameter dependence of the deuteron yield identifying the struck particles with the emitted ones and applying the Sackur-Tetrode formalism to determine the deuteron number. This method, however, relies on the assumption of thermal equilibrium. A new method of calculating the entropy which takes into account correlations will be discussed in this paper.

In Sec. II we describe how the formalism of Refs. 5 and 6 has been adapted to the BUU model. Section III surveys the general features of the 800 MeV Ca + Ca reaction predicted by BUU and shows the comparison to data. In Sec. IV we investigate the dependence of the deuteron to proton ratio on the nuclear equation of state. There are two important questions involved: (1) Do deuterons carry information about the state at highest density? (2) Is the d/p ratio sensitive to the equation of state? We will show using a simple estimate that one should not expect much sensitivity, and will compare this prediction with the results given by our solutions to the BUU equation. Section V treats entropy production, and Sec. VI is a summary.

II. THEORY

For the derivation of the BUU equation and details of its numerical solution the reader is referred to Ref. 8 and the references therein. The theory relating phase space distributions and inclusive fragment cross sections is discussed in Refs. 5, 6, and 13. Here we briefly describe how the deuteron cross section was calculated in the context of the BUU approach.

Each BUU simulation provides the following approximation to the Wigner representation of the full density operator:

$$\rho_w(t)=\left\langle \prod_1^A h^3\delta[\mathbf{x}_a-\boldsymbol{\kappa}_a(t)]\delta[\mathbf{p}_a-\boldsymbol{\not{k}}_a(t)]\right\rangle , \tag{2.1}$$

where $(\mathbf{x}_a,\mathbf{p}_a)$, $a=1,\ldots,A$, are the phase space variables of the density operator in the Wigner representation for the A-body system, $[\boldsymbol{\kappa}_a(t),\boldsymbol{\not{k}}_a(t)]$ are their time-dependent trajectories, $h=2\pi$ is Planck's constant in the units we are using, and $\langle\cdots\rangle$ signifies an ensemble average over the trajectories generated in a BUU simulation. In both a BUU and an INC model calculation, $[\boldsymbol{\kappa}_a(t),\boldsymbol{\not{k}}_a(t)]$ for each particle (a) describes its trajectory in its own six-dimensional phase space. In an INC calculation this trajectory is a sequence of straight line segments; each segment describes free (ballistic) motion of the particle between its consecutive (two-body) collisions with neighboring particles. In BUU calculations there are two major differences: (1) Each segment is curved by the mean field. (2) Each collision is moderated by Pauli blocking.

The general theory of composite fragment production when applied to the INC model[6] leads to the following expression:

$$N_D'=\tfrac{3}{4}\left\langle \sum_{\mathrm{n,p}}\sum_t \delta[\mathbf{p}-\boldsymbol{\not{k}}_{\mathrm{np}}(t+)]D(t+) -\delta[\mathbf{p}-\boldsymbol{\not{k}}_{\mathrm{np}}(t-)]D(t-)\right\rangle , \tag{2.2}$$

where the $\sum_{\mathrm{n,p}}$ means a sum over all neutron-proton pairs in the system, $\sum_t$ means a sum over all (discrete t) collision times of the pair with a third body (a collision of either member counts as a collision of the pair), $\boldsymbol{\not{k}}_{\mathrm{np}}(t+)=\boldsymbol{\not{k}}_{\mathrm{n}}(t+)+\boldsymbol{\not{k}}_{\mathrm{p}}(t+)$ is the total momentum of the pair immediately after the collision at t (*mutatus mutandis* for $t-$ before collision), and

$$D(t+)=D(\boldsymbol{\kappa}_{\mathrm{n}}(t+)-\boldsymbol{\kappa}_{\mathrm{p}}(t+),[\boldsymbol{\not{k}}_{\mathrm{n}}(t+)-\boldsymbol{\not{k}}_{\mathrm{p}}(t+)]/2) , \tag{2.3}$$

where $D(\mathbf{x},\mathbf{p})$ is the Wigner function describing the deuteron bound state. N_D' is the number of primordial deuterons observed per volume element in momentum space. Primes are used to emphasize that what are being referred to here are "primordial" deuterons as opposed to true or observed deuterons. Roughly speaking, primordial deuterons consist of all np pairs which find themselves in deuteronlike correlations in the final state. Their number therefore includes not only observed deuterons but also contributions from such correlations in larger nuclei.

The $t+$ term in Eq. (2.2) can be interpreted as meaning that a primordial deuteron can only be formed from a pair of particles when one member of the pair collides with a third particle. This is, of course, in accord with the fact that two free nucleons by themselves cannot coalesce into a bound state. The probability for formation is given by the overlap between the phase space distribution representing the deuteron and that representing the np pair after collision. Similarly, the $t-$ term corresponding to the time-reversed process, primordial deuteron annihilation, requires a third particle to catalyze it. In the BUU model, each member of a pair interacts with neighboring particles not only by collision but also via the mean field which then ought to also catalyze primordial deuteron production and annihilation. Unfortunately, the equation corresponding to Eq. (2.2) for the BUU model, which would take into account this extra mode of catalysis, has not yet been derived. In this paper we have therefore simply used Eq. (2.2).

The adoption of the INC model's Eqs. (2.2) for BUU has necessitated yet another approximation. For large impact parameter collisions in BUU, two heavy spectator fragments survive which are bound with low excitation by their respective mean fields. Nucleons from them can contribute to N_D' either through evaporation or by being picked up by participant nucleons. Since Eq. (2.2) is not adequate to treat these processes, we have only used it with nucleons which are not bound in spectators at the end of a simulation. The major error due to this will be in regions of the spectra where fragments move near spectator velocities.

III. RESULTS

We performed calculations for the reaction 800 MeV/nucleon Ca + Ca. This system was measured by Nagamiya *et al.*,[10] and deuteron spectra are available for a wide kinematic range. One hundred simulations were run at each of nine different impact parameters. Our calculation reproduces the total number of impact parameter

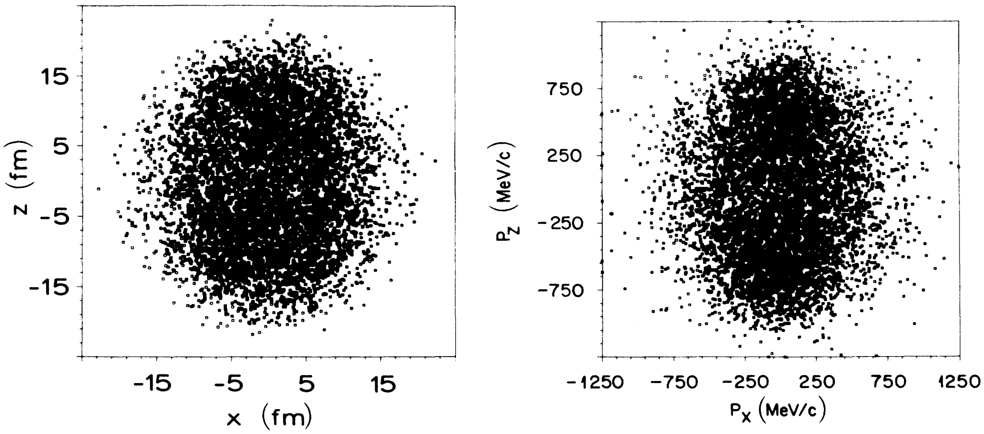

FIG. 1. Density profile of the reaction of 800 MeV/nucleon Ca + Ca at $b=0$ fm. On the left, the coordinates of all 8000 particles at $t=60$ fm/c are projected onto the xz plane, where z is the beam axis and x is the direction of the impact parameter. On the right, the final momentum space is projected onto the p_xp_z plane.

averaged evaporated charges reported in Ref. 10 (experiment ~10, BUU calculation ~11.8). This number approximates the number of participant protons. However, our calculation shows that only ~75% of evaporated particles come from geometrical overlap. Large impact parameter collisions led to two heavy, low excitation spectator fragments whose nucleons were assumed not to contribute to deuteron production.

A. The phase space distribution

Figure 1 shows the distribution of nucleons in position and momentum recorded at the final simulation time of 140 fm/c for a central collision. In the momentum distribution we see basically two domains: a strongly populated midrapidity region and remnants of the Fermi spheres of the projectile and the target. In particular, complete equilibriation, which would result in an isotropic distribution, both of these nucleons and of the fragments they form in the final state, is not observed. We want to mention the striking similarity between this reaction and that of 84 MeV/nucleon C + C (Refs. 8 and 11), and the clear difference between these and the 25 MeV/nucleon O + C reaction. Thus after some point near 84 MeV/nucleon, there appears to be little qualitative change in this distribution over one order of magnitude in bombarding energy.

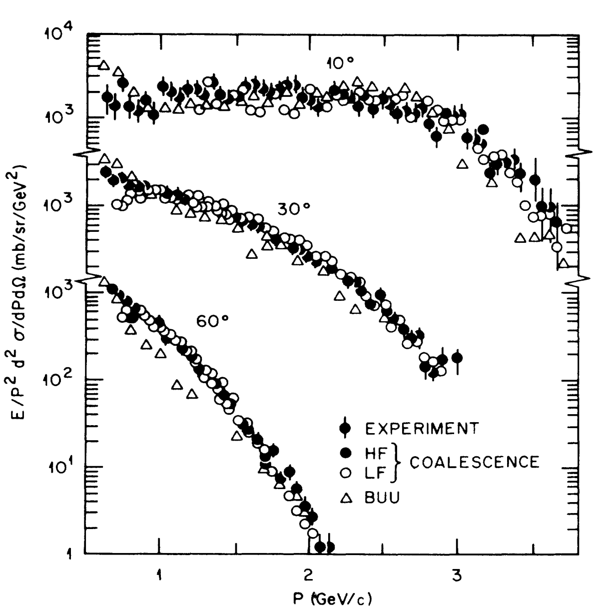

FIG. 2. The deuteron distribution at forward angles in the 800 MeV/nucleon Ca + Ca reaction, comparing our prediction with experimental data and the prediction of other models.

B. The deuteron spectrum

Figure 2 shows the measured deuteron distribution[10] and the calculated distribution of deuteronlike correlations (primordial deuterons). It should be borne in mind

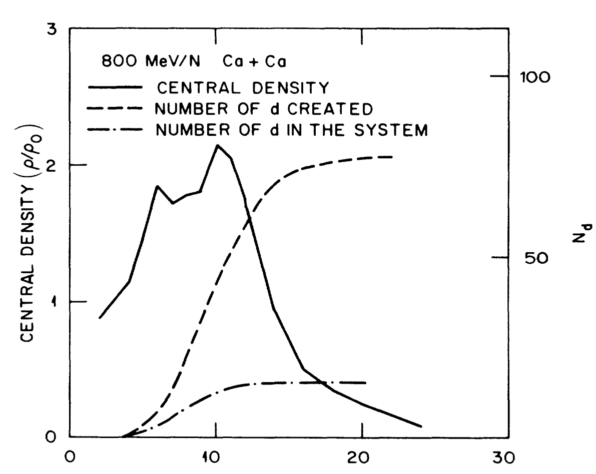

FIG. 3. Central density, the number of deuterons produced, and the number of deuterons in the system as a function of time.

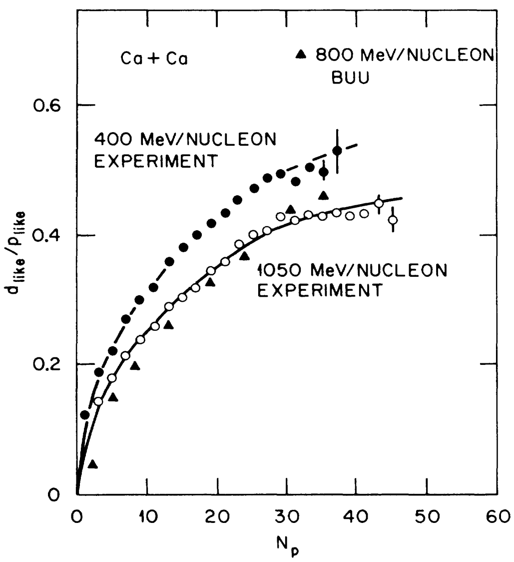

FIG. 4. Deuteron to proton ratio as a function of the charge multiplicity in the reaction Ca + Ca comparing experimental data at 400 MeV/nucleon and 1050 MeV/nucleon with the BUU calculation at 800 MeV/nucleon.

that the calculations contain no adjustable parameters. (The function D representing the deuteron was kept the same as in Ref. 6.) Theoretically, the difference between primordial and measured deuterons is important mainly at low momenta and typically accounts for up to a 50% correction.[6] It seems probable that the very low momentum discrepancy in Fig. 2 is a result of this.

At larger momenta, especially at 60 deg, predicted values appear low. This could be due in part to off-shell scattering mechanisms not sufficiently accounted for in the BUU model. For example, the momentum of quasielastically produced deuterons[14] produced at 30 and 60 deg at this bombarding energy is 1.5 GeV/c and 0.8 GeV/c, respectively, and especially at 60 deg their cross section is large enough to have an appreciable effect. These deuterons come from three nucleons interacting simultaneously at short range. This involves high momentum transfer off-shell collisions not included in mean field effects. Furthermore, this is but one example of a large class of similar mechanisms not included in BUU which, while not important in terms of overall quantities of nucleons they effect, can significantly alter large momentum transfer portions of the spectrum. It should also be remembered that our theoretical statistics deteriorate at low cross-section portions of the spectra.

C. The time evolution of primordial deuterons

Figure 3 displays the central density and the gross and net numbers of primordial deuterons produced versus time for central collisions. We see that in this (light) system the central density does not exceed twice that of normal nuclear matter. This disagrees with INC calculations which exhibit almost twice as much compression, and therefore demonstrates the strong influence of the mean field even at relatively high bombarding energies.

The figure also shows that a large fraction of primordial deuterons are produced near maximum compression. By maximum compression, the net primordial deuteron curve has saturated, i.e., production and destruction rates are balanced. The gross production rate falls rapidly as the system decompresses. (Curves with similar information based on a simplified fluid dynamical model may be found in Ref. 13.) These results suggest that deuterons carry information about the high compression phase, a possibility which we will discuss in more detail in Sec. IV.

D. Impact parameter dependence

The impact parameter dependence of deuteron production has not previously been well studied. Model calculations of various quantities (e.g., freeze-out density, entropy, or coalescence radius) have usually assumed that these quantities are insensitive to impact parameter (see, however, Ref. 4). Recently published experimental data[12] indicate that primordial deuteron/proton ratios vary strongly with total multiplicity and hence with impact parameter. These measurements also support the assumption that the deuteron yield is roughly proportional to the square of the participant proton yield. Figure 4 shows the comparison between our results and these experimental values obtained at 400 and 1050 MeV/nucleon. Although one must be cautious because we did not apply the filter routines for the plastic ball data, we see good agreement between theory and experiment regarding both the absolute magnitudes and general trend of these values.

E. Implications for fireball model

As already pointed out, a globally equilibriated fireball is not obtained in this reaction. One can define, nonetheless, effective longitudinal and transverse temperatures for emitted particles. Particles coming from the geometrical overlap region are found to have temperatures of 170 MeV and 75 MeV in these directions, respectively, while the remainder have 66 MeV and 47 MeV. These temperatures are found to be independent of impact parameter. In the fireball model, the deuteron-proton ratio is related to the freeze-out density, which determines when the system switches from thermal equilibrium to free expansion. The freeze-out density is given by

$$\rho = \tfrac{4}{3} N_D / N_N (MT/2\pi)^{3/2} = \text{const} \times N_D / N_N \ . \quad (3.1)$$

As one can see from Table I, ρ varies significantly with impact parameter. Therefore, freeze-out densities extracted from impact parameter averaged data have no physical meaning but are only parametrizations of the data. Furthermore, we note that

$$\langle N_D / N_N \rangle \neq \langle N_D \rangle / \langle N_N \rangle \ .$$

IV. SENSITIVITY OF d/p RATIO TO EQUATION OF STATE

The sensitivity of N_D/N_P to the nuclear equation of state was investigated by running the simulation with two

TABLE I. Impact parameter dependence of different quantities. The first and second columns show the impact parameter and the cross section represented by the simulation of the reaction at this impact parameter. The third through seventh columns represent the number of protonlike clusters (total emitted charge), deuteronlike clusters, the ratio at both values, and the average phase space density at 25 fm/c, respectively. The last three columns present the entropy per baryon using Eqs. (5.1), (5.2), and (5.3), respectively.

b (fm)	σ (mb)	N'_P (BUU)	N'_D (BUU)	N'_P/N'_D	$\langle n \rangle$ (BUU)	$S/N=3.95-\ln\frac{N'_D}{N'_P}$	S_{Boltz}/N	S/N (including compressibility)
1.4	122	30.2	12.7	0.42	0.044	4.8	4.5	5.0
2.4	122	23.7	8.3	0.35	0.035	5.0	4.8	5.3
3.1	122	19.3	6.3	0.32	0.030	5.1	5.1	5.5
3.7	122	15.6	3.3	0.21	0.025	5.5	5.2	5.6
4.2	122	12.3	3.1	0.26	0.021	5.3	5.6	6.0
4.6	122	8.4	1.5	0.18	0.020	5.7	5.8	6.1
5.4	366	5.2	0.8	0.15	0.015	5.8	6.2	6.6
6.4	366	2.0	0.08	0.04	0.007	7.1	7.1	7.2
7.3	366	0.5	0.02	0.035	0.004	7.3	8	8.1
	σ_{tot}2196							
ϕ		8.8	2.5			6.1	6.3	6.6

different potential energy functions of the form $U=a\rho+b\rho^c$, where ρ is the density in units of 0.15 nucleons/fm,^{3} $a=-356$ (-124), $b=303$ (70.5) (in MeV), and $c=\frac{7}{6}(2)$. These have isothermal compressibilities (at zero temperature and $\rho=1$) of 380 (200) MeV and therefore give rise to rather different equations of state which we denote as stiff (soft). Despite this, we get a primordial deuteron ratio of only $N'_D(\text{stiff})/N'_D(\text{soft})=1.1$. This result can be qualitatively understood using the fact that the maximum central density attained by the system was also found to be insensitive to compressibility; for either equation of state it came out to be about twice normal nuclear matter. At this density, $U(\text{stiff})-U(\text{soft})\sim 12$ MeV, which in turn leads to the estimate $T(\text{soft})/T(\text{stiff})\sim\frac{117}{124}$. Since phase space volume goes as $T^{3/2}/\rho$, an overlap estimate of primordial deuterons gives

$$N'_D(\text{stiff})/N'_D(\text{soft})=T(\text{stiff})/[T(\text{soft})]^{-3/2}=1.1$$

(the larger the volume the less the probability for two nucleons to overlap to form a primordial deuteron).

Since compression increases with the net mass of participants, these considerations also imply that impact parameter averaged d/p ratios will be even less sensitive to the equation of state than central collisions. In any case, even 10% effects are too small to be seen given present experimental and theoretical uncertainties so that our main conclusion must be that the d/p ratio cannot at present provide direct information concerning compressibility and its related equation of state.

However, these same considerations also suggest ways to enhance sensitivity to compressibility. First, one should look at collisions between heavier systems since these will achieve greater compression and hence a greater difference between stiff and soft temperatures. Second, one should look at the dependence of heavier composite formation on compressibility, since, using the same arguments as for deuterons, these should depend more strongly on temperature, going roughly as $N_A\sim T^{-1.4(A-1)}$.

V. ENTROPY PRODUCTION

Siemens and Kapusta[1] attempted the first estimate of entropy production. Their highly idealized model assumes that at some time during expansion, nuclear matter can be treated as a dilute gas of mainly nucleons and deuterons in local chemical equilibrium. Assuming equal numbers of neutrons and protons and a temperature much greater than deuteron binding, the entropy per nucleon according to the statistical mechanics of perfect gases is

$$S/N=3.95-\ln(N_D/N_P)\,. \tag{5.1}$$

Subsequently, Bertsch and Cugnon[7] derived a similar formula in which N_D/N_P gets replaced by N'_D/N'_P, the primordial deuteron proton ratio. It avoids, to some extent, reliance on chemical equilibrium and diluteness but makes a number of other assumptions whose validity is hard to estimate. In the same paper, a calculation of the Boltzmann form of the entropy

$$S_{\mathrm{Boltz}}/N=-\int d\mathbf{x}\,d\mathbf{p}(2\pi)^{-3/2}n(\mathbf{x},\mathbf{p})[\ln n(\mathbf{x},\mathbf{p}/4)-1] \tag{5.2}$$

was made, based on an intranuclear cascade simulation. Here, n is the single nucleon distribution function in phase space evaluated after the last collision in the simulation. Equal numbers of protons and neutrons are assumed. Note that the Boltzmann entropy equals the true entropy only in the absence of multiparticle correlations and this method of calculating it of course depends entirely on the validity of the intranuclear cascade model itself. Recently it was shown[17] that the prescription of Bertsch and Cugnon overestimates the entropy by more than half a unit.

A more recent paper[15] attempts to free the measurement of entropy produced during a collision from extraneous assumptions as much as possible. Briefly, it is based on the following: (1) The entropy of a colliding system is well defined and asymptotically approaches a time-independent "collisional" entropy as the system separates. (2) Collisional entropy is a function of only the final state of the system. Out of all possible (mixed) states agreeing with some set of measured final state observables, there is a unique one of maximum entropy which is therefore an upper bound to the collisional entropy. (3) The more experimental information delimiting the maximum entropy, the lower it is. (4) One can never do better than finding an upper bound to collisional (or in fact any) entropy since any correct estimate should be unbiased and any unbiased estimate must give an upper bound. This is because an unbiased statistical ensemble specified by average values of a set of observables always has (by definition) an entropy which is larger than that of a biased ensemble satisfying the same specifications.

If we choose the single particle distributions $n_\tau(\mathbf{x},\mathbf{p})$ for all final state reaction products τ evaluated at any time after interactions have ceased as the set of observables defining the maximum entropy state, then one can show[15] that this state's entropy per nucleon is time independent and given by

$$S/N=-\sum_\tau \int d\mathbf{x}\,d\mathbf{p}/(2\pi)^3 n_\tau(\mathbf{x},\mathbf{p}) \times[\ln(n_\tau(\mathbf{x},\mathbf{p})/g_\tau)-1]\ , \qquad (5.3)$$

where g_τ is the degeneracy. Note that Eq. (5.3) does not depend on any equilibrium or spatial diluteness assumptions and the particles referred to are *not* primordial. This upper bound could in principle be improved by taking more than the single particle distributions into account (e.g., correlations among produced fragments) but even this formula requires more information than is presently available from simulations (experiment cannot directly provide the spatial dependence in the n_τ). As a first try we have therefore simply guessed at the spatial distribution using the prescription

$$n_\tau(\mathbf{x},p)\simeq c\,[n_{\mathrm{BUU}}(\mathbf{x},\mathbf{p}/A)]^A\ , \qquad (5.4)$$

where $A=A_\tau$ is the number of nucleons in τ and $c=c_\tau$ is a normalization constant determined by fitting total yields of the τ to data. The distribution n_{BUU} is that of the primordial nucleons at the end of the BUU calculation; assuming that they propagate freely after this time, Eq. (5.4) has the correct time dependence for freely propagating τ, and hence the entropy calculated using it is the same at any later time. The observed nucleon distribution is then taken to be

$$n_N(\mathbf{x},\mathbf{p})\simeq n_{\mathrm{BUU}}(\mathbf{x},\mathbf{p})-\sum_\tau A n_\tau(\mathbf{x},\mathbf{p}/A)\ , \qquad (5.5)$$

where, in this calculation, the sum is extended through ^{4}He.

There are a number of uncertainties and ambiguities in the use of Eqs. (5.4) and (5.5). A more accurate procedure[15] was developed subsequent to this calculation and has not yet been implemented. Thus, despite its deficiencies, this is probably the best calculation currently available. Table I gives the results for all three methods discussed. Comparison of the last three columns teaches us two things: (1) Entropy increases strongly with impact parameter in all methods. It is therefore incorrect to attempt an entropy measurement without taking this into account. In particular, naive use of impact parameter averaged data is certain to be in gross error. (2) Entropy values differ between these methods, typically at the 0.3–0.5 level at all energies. This corresponds to a factor of $\sim e^{40}$ in total phase space volume. Since all these methods involve very different (generally incorrect) assumptions, we conclude that until the procedures in (Ref. 15) have been implemented, nothing of possible interest can be deduced from such calculations.

VI. SUMMARY

We have calculated deuteron production using the BUU model for the time-dependent single nucleon density and the correct scattering theory expression for relating it to the deuteron production rate. Our results are in good agreement with the data in both absolute value as well as in spectral shape. We find that the freeze-out density is a rather artificial quantity which cannot be related to an actual density of the system. We also find that entropy cannot be meaningfully measured using currently available techniques.

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