On the Information Content of the One-Body Density

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1. Introduction

Before two heavy ions collide they are assumed to be in their ground state and the relative motion can be regarded as a wave packet. Thus the whole system is prepared in a pure state. After the collision the system is highly excited and the measured data can be described best by a mixed state (statistical operator). During the reaction the system is closed and there is no external heat bath which could absorb information and give rise to a mixed state. It is rather the incomplete measurement which implies a loss of information and hence entropy production.

In this work we assume that the observer can measure the expectation values of all one-body operators. This is certainly much more information than can be achieved in heavy ion collisions. It is however just the information which equations of motion for the one-body density matrices are dealing with. We shall first construct the statistical operator of maximum entropy under the constraint of a given one-body density. From this we deduce the entropy and the two-body density matrix. We distinguish between the "grand canonical" ensemble and the one where the total number of particles is known. The two-body density of maximum entropy is applied to a model case and to heavy ions in thermal equilibrium.

2. The concept of maximum entropy

A formal way to reduce the information is the concept of maximum entropy [Ka67]. Assume the information I about the systems to be contained in a set of operators B_α and their expectation values.

$$I = \left\{ B_\alpha \, , \langle B_\alpha \rangle ; \; \alpha = 1, \dots, N \right\} \tag{1}$$

Then the statistical operator R given in eq. 2 is the one of maximum entropy among all others which yield a given set of expectation values $\langle B_\alpha \rangle$.

$$R = e^{-\sum_{\alpha=1}^{N} \lambda_\alpha B_\alpha} \tag{2}$$

$$\langle B_\alpha \rangle = \mathrm{Tr}\,(R B_\alpha) = \langle \Psi | B_\alpha | \Psi \rangle \tag{3}$$

The Lagrange parameters $\lambda_\alpha(t)$ have to be determined such that eq. 3 is fulfilled for $\alpha = 1, \dots, N$. It is furthermore assumed that the expectation values are the same as for the exact state $|\Psi\rangle$ (eq. 3). The entropy S belonging to R is given by

$$S = -\mathrm{Tr}\,(R \ln R) = \sum_{\alpha=1}^{N} \lambda_\alpha \langle B_\alpha \rangle \tag{4}$$

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The statistical operator R can also be regarded as the result of a projection of the pure state $|\Psi\rangle\langle\Psi|$ [Ro66]

$$|\Psi\rangle\langle\Psi| \xrightarrow{\;\mathcal{P}\;} R \tag{5}$$

One can of course calculate any other expectation value $\langle x\rangle = \mathrm{Tr}(Rx)$ with this statistical operator. If it turns out that $\langle x\rangle \approx \langle\Psi|\, x\, |\Psi\rangle$ it is said that $\{x,\langle x\rangle\}$ does not contain new information which is not already in the set I. If $\langle x\rangle$ differs significantly from the exact result (or measurement) $\{x,\langle x\rangle\}$ is informative and has to be included in I.

We want to follow these ideas by assuming the one-body information to be essential and construct at each time t R(t), determine the entropy S(t), and the two-body density [Fe81].

For a given single-particle basis

$$|\widetilde{\alpha,1}\rangle := \tilde{a}^+_\alpha |0\rangle \tag{6}$$

the one-body density matrix is defined as

$$\tilde{\rho}^{(1)}_{\alpha\beta}(t) = \langle\Psi(t)|\, \tilde{a}^+_\beta\, \tilde{a}_\alpha\, |\Psi(t)\rangle \tag{7}$$

If we suppose the system to have a definite particle number A, the information set is

$$I = \left\{ P\,\tilde{a}^+_\beta\,\tilde{a}_\alpha P\,,\; \tilde{\rho}^{(1)}_{\alpha\beta}(t)\;;\; \alpha,\beta = 1,\dots,N \right\}, \tag{8}$$

where P projects on the subspace with particle number A.

$$P = \sum_s |\widetilde{s,A}\rangle\langle\widetilde{s,A}| \tag{9}$$

$|\widetilde{s,A}\rangle$ are Slater determinants created with A operators $\tilde{a}^+_\alpha$. The statistical operator of maximum entropy is herewith given by

$$R(t) = \sum_{ss'} |\widetilde{s,A}\rangle\langle\widetilde{s,A}|\, e^{-\sum_{\alpha\beta}\lambda_{\alpha\beta}(t)\tilde{a}^+_\beta\tilde{a}_\alpha}\, |\widetilde{s',A}\rangle\langle\widetilde{s',A}| \tag{10}$$

It is more convenient to transform $\tilde{\rho}^{(1)}_{\alpha\beta}(t)$ into its eigenbasis

$$\rho^{(1)} = \sum_{\alpha\beta} |\widetilde{\alpha,1}\rangle\, \tilde{\rho}^{(1)}_{\alpha\beta}(t) \langle\widetilde{\beta,1}| = \sum_\alpha |\alpha,1\rangle_t\, \rho^{(1)}_{\alpha\alpha}(t)\; {}_t\langle\alpha,1| \tag{11}$$

and to represent R(t) with Slater determinants $|s,A\rangle_t$ built out of the single-particle states $|\alpha,1\rangle_t$ which depend on time however. In the following we omit the time argument again. With

$$a^+_\alpha |0\rangle = |\alpha,1\rangle \tag{12}$$

and $$B_\alpha = a_\alpha^+ a_\alpha \tag{13}$$

we get $$R = \sum_s |s,A\rangle \, e^{-\sum_\alpha \lambda_\alpha b_\alpha^{(s)}} \langle s,A| \, . \tag{14}$$

$b_\alpha^{(s)}$ are the occupation numbers in $\langle s,A|$:

$$B_\alpha \, |s,A\rangle = b_\alpha^{(s)} \, |s,A\rangle \tag{15}$$

If we drop the condition of sharp particle number we consider the information I_{GC} equivalent to the grand canonical ensemble:

$$I_{GC} = \left\{ \tilde{a}_\alpha^+ \tilde{a}_\beta \, , \, \tilde{\rho}_{\alpha\beta}^{(1)} \, ; \, \alpha,\beta = 1,\ldots,N \right\} \tag{16}$$

The statistical operator of maximum entropy becomes [Wi63]

$$R_{GC} = \frac{1}{Z_{GC}} e^{-\sum_{\alpha\beta} \chi_{\alpha\beta} \tilde{a}_\beta^+ \tilde{a}_\alpha} = \frac{1}{Z_{GC}} e^{-\sum_\alpha \lambda_\alpha a_\alpha^+ a_\alpha} \tag{17}$$

Especially the partition sum Z_{GC} assumes a simple form

$$Z_{GC} = \sum_{s,A} e^{-\sum_\alpha \lambda_\alpha b_\alpha^{(s)}} = \prod_\alpha \left(1 + e^{-\lambda_\alpha}\right) \tag{18}$$

Also the relation between the Lagrange parameter and the mean occupation numbers can be given analytically

$$\lambda_\alpha = \ln \frac{1 - \rho_{\alpha\alpha}^{(1)}}{\rho_{\alpha\alpha}^{(1)}} \quad . \tag{19}$$

Using eq. 4 for the entropy we get

$$S_{GC} = - \sum_\alpha \left\{ \rho_{\alpha\alpha}^{(1)} \ln \rho_{\alpha\alpha}^{(1)} + \left(1 - \rho_{\alpha\alpha}^{(1)}\right) \ln \left(1 - \rho_{\alpha\alpha}^{(1)}\right) \right\} \tag{20}$$

Eq. 20 is exact and one does not need Stirling's formula to derive it, as done in [LF75].

3. Maximum entropy two-body density matrix

Utilizing the statistical operator given in eq. 14 or eq. 17 we can calculate the two-body density matrix as

$$\rho_{\alpha\beta\gamma\delta}^{(2)} = \mathrm{Tr}\left(R \, a_\delta^+ a_\gamma^+ a_\alpha a_\beta \right) \tag{21}$$

Choosing the representation in which $\rho^{(1)}$ is diagonal we get for the sharp particle number case

$$\rho_{\alpha\beta\gamma\delta}^{(2)} = \left(\delta_{\alpha\gamma} \delta_{\beta\delta} - \delta_{\alpha\delta} \delta_{\beta\gamma} \right) \sum_s b_\alpha^{(s)} b_\beta^{(s)} e^{-\sum_\varepsilon \lambda_\varepsilon b_\varepsilon^{(s)}} \tag{22}$$

The sum over s has to be performed for all possible Slater determinants with A particles. If we are dealing with N single-particle levels the sum has $\binom{N}{A}$ terms. For large A and N the summation becomes rather expensive. Therefore we propose in the following an approximation to eq. 22 relating $\rho^{(2)}$ directly to $\rho^{(1)}$. It turned out to work very well in cases where the sum (22) could be evaluated. The partition sum is given by

$$Z = \sum_s e^{-\sum_\alpha \lambda_\alpha b_\alpha^{(s)}} \tag{23}$$

The one-body density can be regained from Z by

$$\rho^{(1)}_{\alpha\alpha} = -\frac{1}{Z}\frac{\partial Z}{\partial \lambda_\alpha} \tag{24}$$

Similarly the two-body density is given by

$$\rho^{(2)}_{\alpha\beta\alpha\beta} = \frac{1}{Z}\frac{\partial^2 Z}{\partial\lambda_\alpha\partial\lambda_\beta}(1-\delta_{\alpha\beta}) = \left\{\rho^{(1)}_{\alpha\alpha}\rho^{(1)}_{\beta\beta} - \frac{\partial}{\partial\lambda_\alpha}\rho^{(1)}_{\beta\beta}\right\}(1-\delta_{\alpha\beta}) \tag{25}$$

The approximation consists in replacing $(\partial/\partial\lambda_\alpha)\rho^{(1)}_{\beta\beta}$ which is equal to $(\partial/\partial_{\lambda\beta})\rho^{(1)}_{\alpha\alpha}$ by a product of yet unknown numbers $\mu_\alpha\mu_\beta$

$$\rho^{(2)}_{\alpha\beta\alpha\beta} \approx \left\{\rho^{(1)}_{\alpha\alpha}\rho^{(1)}_{\beta\beta} - \mu_\alpha\mu_\beta\right\}(1-\delta_{\alpha\beta}) \tag{26}$$

The μ_α guarantee the two-body density to reduce properly to the given one-body density

$$\sum_\beta \rho^{(2)}_{\alpha\beta\alpha\beta} = (A-1)\,\rho^{(1)}_{\alpha\alpha} \tag{27}$$

Using eq. 27 we get a system of coupled quadratic equations

$$\mu_\alpha\left(\sum_\beta \mu_\beta - \mu_\alpha\right) = \rho^{(1)}_{\alpha\alpha}\left(1-\rho^{(1)}_{\alpha\alpha}\right). \tag{28}$$

A formal solution obeying physical conditions on $\rho^{(2)}$ is given by

$$\mu_\alpha = \frac{\gamma}{2}\left(1-\sqrt{1-\frac{4\rho^{(1)}_{\alpha\alpha}(1-\rho^{(1)}_{\alpha\alpha})}{\gamma^2}}\right) \quad \text{with} \quad \gamma = \sum_\beta \mu_\beta \tag{29}$$

γ can be obtained by starting an iteration with $\gamma^2 = \max[4\rho^{(1)}_{\alpha\alpha}(1-\rho^{(1)}_{\alpha\alpha})]$ calculating μ_α/γ via eq. 29, then determining a new γ^2 by

$$\gamma^2 = \frac{\sum_\alpha \rho^{(1)}_{\alpha\alpha}\left(1-\rho^{(1)}_{\alpha\alpha}\right)}{1-\sum_\alpha(\mu_\alpha/\gamma)^2} \tag{30}$$

and so on. Eq. 30 follows by summing eq. 28 over α. The μ_α are different from zero only around the Fermi edge, where $\rho^{(1)}_{\alpha\alpha}$ is in between 0 and 1. All μ_α are zero in the case of a single Slater determinant. Thus approximation (26) is exact in this case. It is also exact for the case where all $\rho^{(1)}_{\alpha\alpha}$ are equal.

In the case where only the one-body density is known and hence only the mean value <A> of the particle number (grand canonical) we get the two-body density $\Gamma^{(2)}$ using eq. 25 for Z_{GC} given in eq. 18.

$$\Gamma^{(2)}_{\alpha\beta\alpha\beta} = \rho^{(1)}_{\alpha\alpha}\, \rho^{(1)}_{\beta\beta}\, (1 - \delta_{\alpha\beta}) \tag{31}$$

or in a general representation

$$\tilde{\Gamma}^{(2)}_{\alpha\beta\gamma\delta} = \tilde{\rho}^{(1)}_{\alpha\gamma}\, \tilde{\rho}^{(1)}_{\beta\delta} - \tilde{\rho}^{(1)}_{\alpha\delta}\, \tilde{\rho}^{(1)}_{\beta\gamma} \tag{32}$$

However, the grand canonical two-body density does not reduce properly to the given one-body density.

$$\sum_{\beta} \Gamma^{(2)}_{\alpha\beta\alpha\beta} = \left(\langle A \rangle - \rho^{(1)}_{\alpha\alpha} \right) \rho^{(1)}_{\alpha\alpha} \tag{33}$$

The lack of information about the mass number results in a fluctuation of this quantity with a width

$$\sigma_A^2 = \left\langle \left(\sum_{\alpha} a^+_\alpha a_\alpha \right)^2 \right\rangle - \left\langle \sum_{\alpha} a^+_\alpha a_\alpha \right\rangle^2 = \sum_{\alpha} \rho^{(1)}_{\alpha\alpha} \left(1 - \rho^{(1)}_{\alpha\alpha} \right) \tag{34}$$

This fluctuation makes the product ansatz (32) worthless for calculating widths of extensive one-body quantities like momentum or mass of a subsystem. The variances will always contain a part which is due to the fluctuating total mass number. The effect is worst if the subsystem contains about half of the matter of the total system and is negligible if the subsystem is small compared to the rest. (See also eq. 42.)

4. Application in a model system

Within the frame of a simplified model [Fe80,BF82] we are going to study the loss of information as seen by an observer who is performing an incomplete measurement. The model describes in one spatial dimension the dynamical evolution of two interpenetrating Fermi gases. The fermions are enclosed in a box and interact via a two-body interaction of finite range. The time-dependent many-body wave function $|\Psi(t)\rangle$ is obtained by solving the Schrödinger equation numerically. A detailed description of this model is given in a contribution by P. Buck and H. Feldmeier [FB82] in these proceedings.

We use the exact wave function $|\Psi(t)\rangle$ and construct the statistical operator of maximum entropy at each time as described in chapter 3. The initial state consists in 4 particles in the left and 6 particles in the right half of the box. At t = 0 the wall separating them is removed instantaneously. We suppose that the observer measures the one-body density matrix. The results are summarized in fig. 1. The entropy S(t) is calculated from eq. 4 and shown in the upper part. At t = 0 the entropy does not vanish since the observer cannot recognize the two-body correlations which are already in the initial state. On the average the entropy increases with time and tends towards the entropy S_K of the canonical distribution for which the

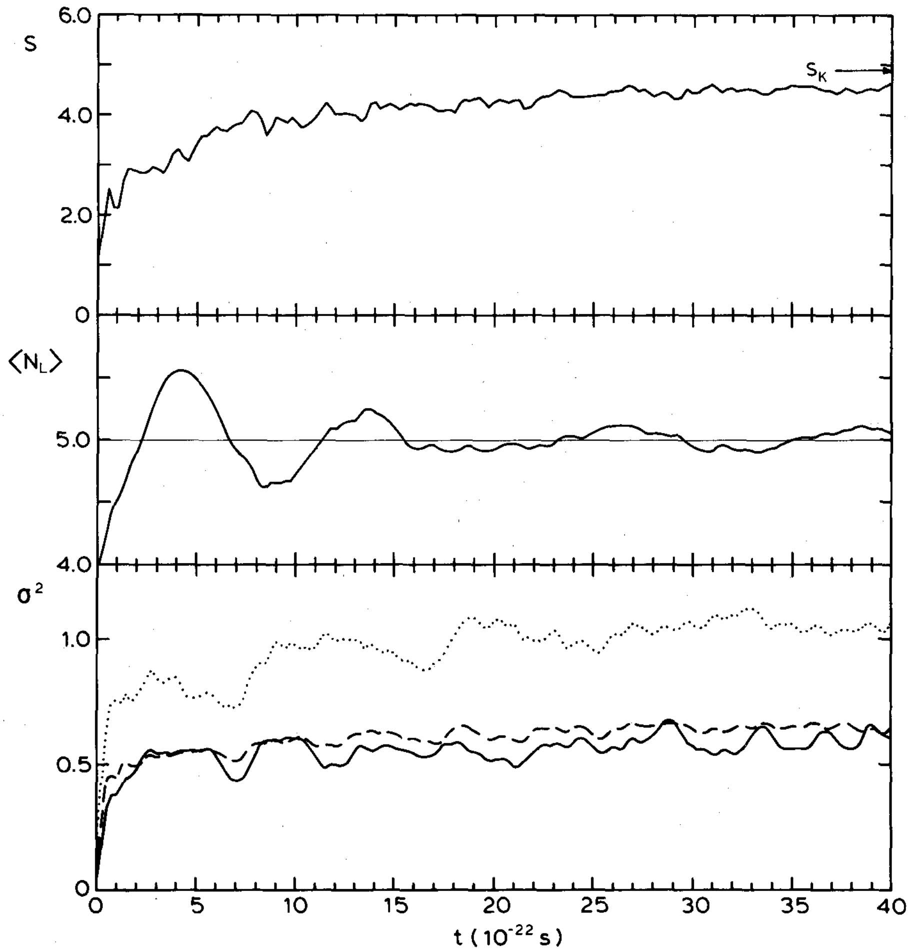

Fig. 1. Dissipative behavior of a model system with a total of 10 fermions (described in more detail in [FB82]). At time t = 0 a wall between 4 particles in the left and 6 particles in the right hand box is removed, giving rise to the time evolution of a wave function. S is the entropy as seen by an observer who measures the one-body density only. $\langle N_L \rangle$ is the mean particle number in the left box and σ^2 is the variance of N_L calculated in three different ways: —— σ^2 exact; ---- σ^2_{ME} deduced from the one-body information; ···· σ^2_{GC} calculated with the product ansatz.

information about the system consists only in knowing the Hamiltonian H and its expectation value or the temperature $1/\beta$.

$$R_K = \frac{1}{Z} e^{-\beta H} \quad ; \quad S_K = \beta \langle H \rangle + \ln Z \tag{35}$$

Eqs. 35 are special cases of eqs. 2 and 4 with $I_K = \{H,1;\ \langle H\rangle, \langle 1\rangle\}$. The unit operator 1 takes care of the normalization. Although physical intuition and Boltzmann's H theorem are in accord with this behavior we think that it is not trivial. The equation of motion is the Schrödinger equation, the state of the system is at any time a wave function, the loss of information is therefore not built into the theory but rather results from an incomplete measurement. There are altogether just 10 particles involved. Our observer who has access only to one-body information would classify the system as dissipative.

The equilibration of the number of particles $\langle N_L\rangle$ on the left side goes along with the saturation of the entropy. The lower part of fig. 1 shows the variances σ^2 of N_L calculated in three different ways. σ^2 denotes the exact variance

$$\sigma^2 = \langle \Psi | N_L^2 | \Psi \rangle - \langle \Psi | N_L | \Psi \rangle^2 \tag{36}$$

σ^2_{ME} is calculated using the statistical operator given in eq. 14 or equivalently the maximum entropy two-body density of eq. 22.

$$\sigma^2_{ME} = \mathrm{Tr}\,(R N_L^2) - (\mathrm{Tr}\,(R N_L))^2 \tag{37}$$

σ^2_{GC} utilizes the product ansatz (eq. 32) or equivalently the "grand canonical" statistical operator R_{GC}.

σ^2_{ME} and σ^2 are close to each other. This allows for our case the conclusion that the one-body information is already enough to calculate the two-body quantity $\langle N_L^2\rangle$. σ^2_{GC} fails completely due to the superposed fluctuation of the total mass number as mentioned previously in chapter 3 (cf. eq. 34). The variance calculated with the approximated $\rho^{(2)}$ (eq. 26) differs so little from σ^2_{ME} that deviations would hardly show up on the graph.

5. Application to heavy ions

Very often in heavy ion physics the two excited nuclei are regarded as a gas of nucleons moving in a mean potential [AS76,GM76,HS76,Ra79] as illustrated in the left part of fig. 2. We are going to take this picture seriously and calculate the variance of the mass distribution. We assume that after the collision when the two nuclei are separated again they have reached thermal and chemical equilibrium. Therefore the mean occupation numbers ρ_α are given in both nuclei by the same Fermi distribution:

$$\rho_\alpha = \left(1 + e^{\frac{\varepsilon_\alpha - \nu}{T}}\right)^{-1} \tag{38}$$

Using the approximation (26) for the maximum entropy two-body density matrix the variance σ^2 is given by

$$\sigma^2 = \sum_{\alpha\in I_L} \left\{ \rho_\alpha(1-\rho_\alpha) - \mu_\alpha\left(\sum_{\beta\in I_L}\mu_\beta - \mu_\alpha\right)\right\} \tag{39}$$

With

$$\gamma_L = \sum_{\alpha\in I_L}\mu_\alpha \quad ; \quad \gamma_R = \sum_{\alpha\in I_R}\mu_\alpha \tag{40}$$

and use of eq. 28 σ^2 can be expressed as

$$\sigma^2 = \gamma_R\,\gamma_L \tag{41}$$

$I_L(I_R)$ denotes the set of states in the left (right) hand nucleus. The further assumptions of level densities $g(\varepsilon_F)$ which are at the Fermi edge proportional to the mass number of the nucleus and low temperature lead to

$$\sigma^2 = \frac{A_L A_R}{A}\,\frac{\gamma^2}{A} \approx \frac{A_L A_R}{A}\,g(\varepsilon_F)\,T \tag{42}$$

A_L and A_R are the mass numbers of the two nuclei. Analyzing eq. 30 it turns out that γ^2 can take values between 0 and A. Thus the first part of eq. 42 implies that the variance cannot exceed the reduced mass of the system (classical limit). The same has been shown to hold for a single Slater determinant [DD79]. It is also valid for a Fermi gas with temperature. Taking all the kinetic energy loss of the heavy ion

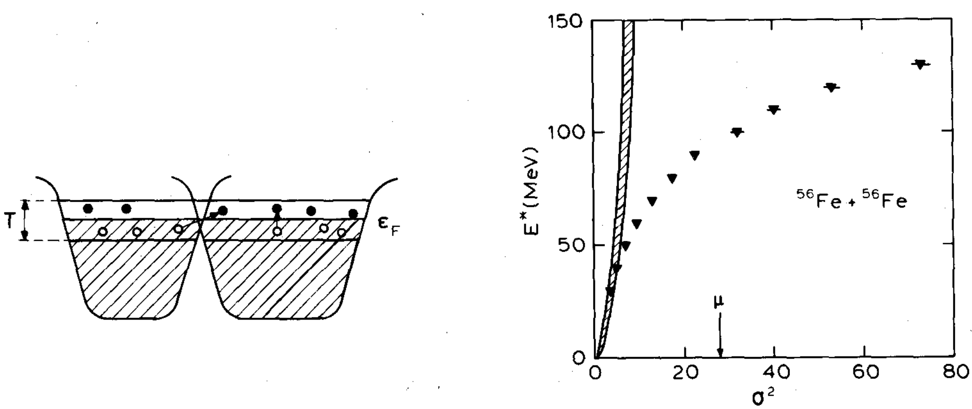

Fig. 2. Schematic of interacting nuclei (taken from [AS76]) and its implication to mass variances measured in heavy ion collisions. The hatched area results from eq. 42 using reasonable level densities $g(\varepsilon_F)$ at the Fermi edge. Triangles are measured data, taken from [BG79].

collision as heat we get the result shown in the right part of fig. 2. The experimental data contradict the assumed physical picture. Since time-dependent Hartree-Fock theories augmented by collision terms are very similar to the picture used here we do not expect them to describe mass fluctuations in heavy ion collisions. (See also [FB82], these proceedings.)

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