

## THE TWO-BODY DENSITY MATRIX OF A SYSTEM IN THERMODYNAMIC EQUILIBRIUM

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A quantity often encountered in nuclear physics, especially when dealing the statistical models of reactions, is the density of energy levels  $dn/dE$ . It is inverse Laplace transform of the partition function of a system:

$$e^{-\beta F} = \int \frac{dn}{dE} e^{-\beta E} dE, \quad \beta = \frac{1}{T}$$

The free energy  $F$  as a function of the temperature  $T$  of a system of  $N$  particles in temperature equilibrium can be calculated directly by requiring  $F = E - TS = \text{minimum}$ . A general way how to solve this equation is to express it in terms of the density matrix  $\hat{\rho}$  of the system:

$$F = \text{Tr } \hat{\rho} \hat{H} + T \text{Tr } \hat{\rho} \ln \hat{\rho} = \text{minimum}$$

and vary  $F$  with the respect to  $\hat{\rho}$ . The explicit solution of this equation

$$\hat{\rho} = e^{\beta(F - \hat{H})}$$

requires the diagonalization of the Hamiltonian in the basis of  $N$ -particles wave functions. For realistic problems this is feasible only in a small model space. The Hamiltonian being usually the two-body operator  $\hat{H}^{(2)}$ , it is possible to express the energy as  $E = \text{Tr } \hat{H}^{(2)} \hat{\rho}^{(2)}$ , where  $\hat{\rho}^{(2)}$  is the two-body density matrix of the system. Since the two-body density matrix is considerably smaller object as the  $N$ -body density matrix it would be tempting to express the entropy  $S$  in terms of the two-body density matrix at least approximately and perform the above calculation using the two-body density matrix elements as variational parameters.

The problem is interesting also from the more general point of view. All the relevant information of a definite state of a system of particles interacting by a two-body force

is contained in the two body density matrix. Since the entropy can be considered as a measure of our information of the system<sup>1,2)</sup>, it is interesting whether it is possible to determine the information contained in the two-body density matrix. The entropy corresponding to the two-body density matrix  $\hat{\rho}^{(2)}$ , we shall call it the two-body entropy  $S^{(2)}$ , can be defined as follows.

A system of  $N$  particles is completely defined by its  $N$ -body density matrix  $\hat{\rho}$ , and its entropy is:

$$S = -\text{Tr } \hat{\rho} \ln \hat{\rho} \quad (1)$$

The relation between  $\hat{\rho}^{(2)}$  and  $\hat{\rho}$ :

$$\hat{\rho}^{(2)}_{ijkl} = \text{Tr } \hat{\rho} \hat{a}_j^+ \hat{a}_i^+ \hat{a}_k \hat{a}_l \quad (2)$$

is not one-to-one. There are several matrices  $\hat{\rho}$  that correspond to the same  $\hat{\rho}^{(2)}$ , so the entropy of the system is not uniquely determined by  $\hat{\rho}^{(2)}$ . But since we are mostly interested in systems having the maximum possible entropy, the following definition seems reasonable:

Let  $\{\hat{\rho}\}$  be the set of all possible  $N$ -body density matrices that give the same  $\hat{\rho}^{(2)}$  and  $\{S(\hat{\rho})\}$  the set of corresponding entropies, then the two-body entropy corresponding to this  $\hat{\rho}^{(2)}$  is equal to the maximum entropy from the set  $\{S(\hat{\rho})\}$ .

We cannot calculate  $S^{(2)}$  directly using the relations (1) and (2). So we present here a suggestion for an approximate relation between the entropy and the two-body density matrix and its test on a soluble model.

We shall make the following approximations and assumptions:

- The conditions which a "representable two-body density matrix should satisfy in order to represent the physical system are not known explicitly. Instead of the set of representable two-body density matrices we choose a somewhat larger set of the two-body density matrices defined by the following necessary conditions: the nonnegativity of the two-body density matrix, the two-hole matrix  $Q_{ijkl} = \text{Tr } \hat{\rho} \hat{a}_j \hat{a}_i \hat{a}_k^+ \hat{a}_l^+$  and the particle hole matrix  $G_{ijkl} = \text{Tr } \hat{\rho} \hat{a}_j^+ \hat{a}_i \hat{a}_k^+ \hat{a}_l$ . The extrem point of this set

have the characteristic property that several eigenvalues of  $\hat{\rho}^{(2)}$ ,  $Q$  and  $G$  matrix are zero. Though these point represent nonphysical states, we believe that they are not too far from the extreme points of the set of the representable two-body density matrices and thus represent a good approximation for exact pure states.

- We require that  $S^{(2)}$  is zero only for approximate pure states having a chosen characteristics number of eigenvalues of  $\hat{\rho}^{(2)}$ ,  $Q$  and  $G$  equal to zero. Let these eigenvalues be  $\lambda_i$  ( $i=1,m$ ).

- For the states inside the set defined above,  $S^{(2)}$  should increase monotonously as  $\lambda_i$  increase.

A possible expression for approximate  $S^{(2)}$  would be:

$$S^{(2)} = -C \sum_{i=1}^m \lambda_i \ln \lambda_i \quad (3)$$

where  $C$  is still an arbitrary constant which our assumptions do not define. A possible way to determine it would be to fit it at the infinite temperature: Consider  $N$  particles distributed among  $L$  single particle states ( $L$  is finite). For the most chaotic ensemble there are  $\left(\frac{L}{N}\right)$  equal possibilities how to distribute them and the entropy is  $S = \ln \left(\frac{L}{N}\right)$ . Computing also the expression  $\sum \lambda_i \ln \lambda_i$  ( $i=1,m$ ) for the ensemble, one can easily determine  $C$ .

We have tested the approximation (3) for the schematic Lipkin's model<sup>3)</sup>, where it is easy to compute the exact  $\hat{\rho}$  and  $\hat{\rho}^{(2)}$ . The model consists of  $N$  fermions located in two  $N$ -fold degenerate levels  $m$  and  $\bar{m}$ . The Hamiltonian looks like:

$$\hat{H} = \frac{\epsilon}{2} \sum_m (\hat{a}_m^+ \hat{a}_m - \hat{a}_{\bar{m}}^+ \hat{a}_{\bar{m}}) + V \sum_{m,n} (\hat{a}_m^+ \hat{a}_n^+ \hat{a}_n \hat{a}_m + \hat{a}_{\bar{m}}^+ \hat{a}_n^+ \hat{a}_n \hat{a}_{\bar{m}}).$$

The comparison of the exact entropy (1) and the approximate two-body entropy (3) for this system in thermodynamic equilibrium is shown for different temperatures and interactions  $V$  on the Figure 1. The calculation of the entropy using the two-body density matrix elements as variational parameters is also presented on the same figure. We have put  $C = 1/7$ .

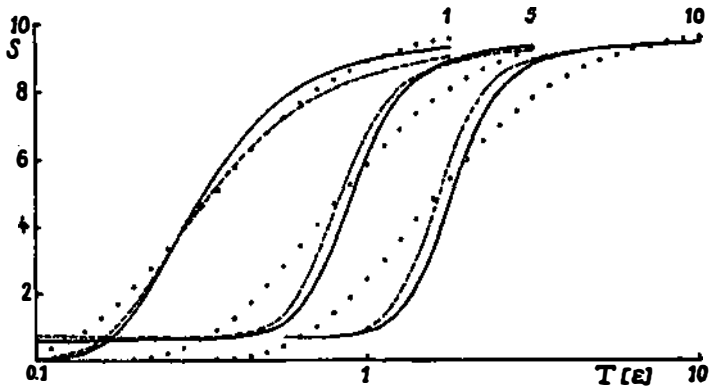


Fig. 1. The comparison between the exact entropy (continuous line), the approximate entropy of the exact two-body density matrix (dashed line) and the entropy from the variational calculation (dots) for Lipkin's model. ( $V=1, 5$  and  $10 \epsilon/N$ ,  $N=8$ )

#### REFERENCES

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