

Reconstruction of quantum states of spin systems via the Jaynes principle of maximum entropy

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Abstract. We apply the Jaynes principle of *maximum entropy* for the partial reconstruction of correlated spin states. We determine the minimum set of observables which is necessary for the complete reconstruction of the most correlated states of systems composed of spins $\frac{1}{2}$ (e.g. the Bell and the Greenberger–Horne–Zeilingger states). We investigate to what extent an incomplete measurement can reveal non-classical features of correlated spin states.

1. Introduction

The seminal paper by Vogel and Risken [1(a)] (see also [1(b)–(j)]) on the tomographic reconstruction of Wigner functions of light fields has greatly enhanced interest into the old problem of ‘measurement’ of states of quantum-mechanical systems. Within the last few years, tomographic reconstruction has been experimentally realized for example by Raymer and co-workers [2] and by Mlynek and co-workers [3]. Tomographic reconstruction schemes of states of other bosonic systems such as vibrational modes of trapped atoms [4] and atomic waves [5] have been proposed. Recently Wigner functions of vibration states of a trapped atom have been experimentally determined by Wineland and co-workers [6], while Kurtsiefer and co-workers [7] have measured Wigner functions of atomic wave packets. Leonhardt [8(a)] (see also [8(b)–(e)]) has extended the ideas of Vogel and Risken to the case of Wigner functions in discrete phase spaces associated with physical systems with finite-dimensional Hilbert spaces, such as spin systems.

The problem of reconstruction of states of finite-dimensional systems is closely related to various aspects of quantum information processing, such as reading of registers of quantum computers [9]. This problem also emerges when states of

atoms are reconstructed. In particular, Walser *et al.* [10(a)] (see also [10(b), (c)]) have shown that, under certain conditions, quantum states of a single quantized cavity mode can be *completely* transferred on to the internal Zeeman submanifold of an atom. Consequently, the reconstruction of the states of a cavity mode is reduced to the problem of reconstruction of angular momentum states in a finite-dimensional Hilbert space.

From the postulates of quantum mechanics it follows that the *complete* reconstruction of a state of a quantum-mechanical system can be performed providing a complete set of system observables (i.e. the *quorum* [11]) is measured on the ensemble of identically prepared systems. On the one hand this goal may be technically difficult to realize and on the other hand it may not be necessary. In many situations even partial knowledge (i.e. incomplete reconstruction) of the state is sufficient for particular purposes.

The complete reconstruction of spin states have been addressed in the literature [8, 11–13]. In the present paper we shall analyse the problem of the partial reconstruction of these states. We shall show how the spin state can be reconstructed when just a restricted set of mean values of the system observables is known from the measurement. Utilizing the Jaynes principle of *maximum entropy* we shall partially reconstruct the density operator from the available (i.e. measured) mean values of system observables.

We shall also address the question which is the minimum observation level (i.e. a specific subset of system observables) on which the complete reconstruction can be performed. In particular, we shall analyse the reconstruction of the most correlated states of the system composed of two and three spins $\frac{1}{2}$ (i.e. the Bell and the Greenberger–Horne–Zeiling (GHZ) states).

The present paper is organized as follows. In section 2 we briefly review the principle of maximum entropy and the formalism of state reconstruction associated with particular observation levels. In section 3 we present a simple illustration of a reconstruction of a state of single spin $\frac{1}{2}$. Section 4 will be devoted to the detailed analysis of the state reconstruction for a system of two correlated spins $\frac{1}{2}$. In section 5 we shall address the problem of the (partial) reconstruction of the GHZ states. In appendix A we present detailed reconstruction of density operators on two non-trivial observation levels.

2. Reconstruction of density operators of quantum states

When it is *a priori* known that experimental data contain the complete information about the state of the system, then it is just a question of technical convenience how to perform a transformation of these data into a more familiar object such as a density operator. A particular example of this procedure is quantum homodyne tomography [1] when from the measured probability distributions of rotated quadratures one can reconstruct[†] (with the help of the inverse Radon transformation) the Wigner function of the state.

Now we can ask the question: ‘What is the density operator of the quantum-mechanical system when an *incomplete* measurement over this system is per-

[†] Strictly speaking, Wigner functions or wave-vectors cannot be measured; they only can be reconstructed from experimental data with the help of some inversion procedures.

formed?’ In this case the experimental data do not provide us with sufficient information to specify the density operator of the system uniquely, that is there can be many density operators which fulfil the constraints imposed by incomplete experimental data. In this situation, one can only *estimate* what is the most probable density operator which describes the system.

In principle we can distinguish two different forms of incompleteness: firstly, when *precise* knowledge of a *subset* of the quorum [11] of system observables is known; secondly, when system observables are not measured precisely, that is instead of probability distributions only frequencies of appearances of eigenvalues of these observables are available.

In the present paper we shall focus our attention on the reconstruction of density operators of spin states when mean values of a subset of system observables are measured precisely. In this case the estimation of density operators can be performed with the help of Jaynes principle of maximum entropy.

2.1. Principle of maximum entropy and observation levels

Let us assume that the state of a spin system, described by the density operator $\hat{\rho}_0$, is unknown and only expectation values G_ν of observables \hat{G}_ν ($\nu = 1, \dots, n$) are available from a measurement. The set of observables is referred to as the *observation level* \mathcal{O} [14]. There can be a large number of density operators $\hat{\rho}$ which are in agreement with the experimental results, that is

$$\text{Tr}(\hat{\rho}\hat{G}_\nu) = G_\nu \quad (\nu = 1, \dots, n). \quad (1)$$

If we wish to use only the expectation values G_ν of the chosen observation level for an estimation (reconstruction) of the density operator, then we face the problem of selecting one particular density operator $\hat{\rho}^\mathcal{O}$ out of many $\hat{\rho}$ which fulfil condition (1). To perform this ‘selection’ (i.e. estimation) we note that the density operators under consideration do differ by their degree of deviation from pure states. To quantify this deviation an uncertainty measure has to be introduced. Following Jaynes [15], one can utilize the von Neumann [16] entropy

$$S[\hat{\rho}] = -\text{Tr}(\hat{\rho} \ln \hat{\rho}). \quad (2)$$

For pure states, $S = 0$ while, for statistical mixtures of pure states, $S > 0$.

According to the Jaynes principle of maximum entropy, we have to choose from a set of density operators $\hat{\rho}$ which fulfil the constraints of equation (1) the generalized canonical density operator $\hat{\rho}^\mathcal{O}$ which maximizes the value of the von Neumann entropy[†]. In other words, the maximum-entropy principle is the *most conservative* assignment, in the sense that it does not permit one to draw any conclusions unwarranted by the measured data. The generalized canonical density

[†] We note that, in principle, instead of the von Neumann entropy one can utilize another uncertainty measure to distinguish between the density operators which fulfil constraints (1). For example, by maximizing the linearized entropy [17]

$$\eta[\hat{\rho}] = 1 - \text{Tr}(\hat{\rho}^2)$$

one can obtain a *partially* reconstructed density operator $\hat{\rho}_\mathcal{O}^{(m)}$ which fulfils conditions (1) and simultaneously leads to the ‘maximum mixture’, that is $\eta[\hat{\rho}_\mathcal{O}^{(m)}] = \max$. Note that, for pure states, $\eta = 0$ while, for mixtures, $\eta > 0$. On the complete observation level, this ‘maximum-mixture’ principle is equivalent to the maximum-entropy principle but, in general, on the reduced (incomplete) observation levels, $\hat{\rho}^\mathcal{O} \neq \hat{\rho}_\mathcal{O}^{(m)}$.

operator (GCDO) $\hat{\rho}^{\mathcal{O}}$ represents a *partially* reconstructed (estimated) density operator on the given observation level \mathcal{O} . The corresponding entropy $S^{\mathcal{O}} = S[\hat{\rho}^{\mathcal{O}}]$ represents the measure of deviation of the reconstructed state from an original pure state. The GCDO $\hat{\rho}^{\mathcal{O}}$ takes the form [14]

$$\hat{\rho}^{\mathcal{O}} = \frac{1}{Z^{\mathcal{O}}} \exp \left(- \sum_{\nu} \lambda_{\nu} \hat{G}_{\nu} \right), \tag{3}$$

$$Z^{\mathcal{O}} = \text{Tr} \left[\exp \left(- \sum_{\nu} \lambda_{\nu} \hat{G}_{\nu} \right) \right],$$

where $Z^{\mathcal{O}}$ is the generalized partition function; λ_{ν} are the Lagrange multipliers which have to be found from the set of equations (1).

Any incomplete observation level \mathcal{O}_A can be extended to a more complete observation level \mathcal{O}_B which includes additional observables, that is $\mathcal{O}_A \subset \mathcal{O}_B$. Additional expectation values can only increase the amount of available information about the state of the system. This procedure is called the *extension* of the observation level (from \mathcal{O}_A to \mathcal{O}_B) and is usually associated with a decrease in the entropy, as $S_B \leq S_A$. We can also consider a *reduction* in the observation level if we decrease the number of independent observables which are measured. This reduction is accompanied with an increase in the entropy due to the decrease in information available about the state of the system. Each incomplete observation level can be considered as a reduction in the complete observation level. In what follows we shall study a sequence of observation levels in the form

$$\begin{aligned} \mathcal{O}_A \subset \mathcal{O}_B \subset \mathcal{O}_C \subset \cdots \subset \mathcal{O}_{\text{comp}}, \\ S_A \geq S_B \geq S_C \geq \cdots \geq 0, \end{aligned} \tag{4}$$

which represent successive extensions of an observation level \mathcal{O}_A towards the complete observation level $\mathcal{O}_{\text{comp}}$.

Concluding this section we make two remarks.

- (1) Firstly we stress that the reconstruction scheme based on the Jaynes principle of maximum entropy does not require any *a priori* assumption about the purity of reconstructed states, that is it can be applied for reconstruction of pure states as well as for statistical mixtures. This reconstruction scheme is equivalent to an averaging over the generalized grand canonical ensemble of *all* states of the system, under the conditions imposed by the constraints given by equation (1). Within the framework of a geometrical formalism, each state of the quantum system is represented by a point in the parametric state space[†]. Those states which fulfil the constraints (1) are represented by a specific manifold in the parametric space. From the maximum-entropy principle it then follows that the generalized canonical density operator is equal to the equally weighted

[†] Pure states, which are elements of the generalized microcanonical ensemble, are represented by points on a manifold in this state space (such as the Poincaré sphere in the case of the spin $\frac{1}{2}$).

average over all states on this specific manifold. Obviously this average is represented by one special point which is associated with the GCDO.

- (2) In the case when there is no information available about the preparation of the system, then there is no intrinsic way to specify the 'minimal' complete observation level. Here by minimal we mean the complete observation level composed of the smallest number of observables. What one can do is to extend systematically observation levels and to evaluate the von Neumann entropy associated with reconstructed GCDOs. If at some stage of the extension of observation levels the von Neumann entropy becomes zero, it then means that the given observation is complete and the pure state of the system is completely 'measured'. Obviously this does not mean that this observation level is minimal[†]. In the case when the measured system is prepared in an unknown statistical mixture it is impossible to specify the minimal observation level until the measurement on the complete observation level has been performed. If this is done, then, by a sequence of reductions under the condition that the von Neumann entropy is unchanged, one can specify the minimal observation level.

In the following sections we shall apply the Jaynes principle for the reconstruction of pure spin states. Firstly, for illustrative purposes we present the simple example of the reconstruction of states of a single spin- $\frac{1}{2}$ system with the help of the maximum-entropy principle. Then we shall discuss the partial reconstruction of entangled spin states. In particular, we shall analyse the problem how to identify incomplete observation levels on which the complete reconstruction can be performed for the Bell and the GHZ states (i.e. the corresponding entropy is equal to zero and the GCDO is identical with $\hat{\rho}_0$).

3. A single spin $\frac{1}{2}$

Firstly we illustrate the application of the maximum-entropy principle for the partial quantum-state reconstruction of single spin- $\frac{1}{2}$ system. Let us consider an ensemble of spins $\frac{1}{2}$ in an unknown pure state $|\psi_0\rangle$. In the most general case this unknown state vector $|\psi_0\rangle$ can be parametrized as

$$|\psi_0\rangle = \cos \theta |1\rangle + \exp(i\varphi) \sin \theta |0\rangle, \quad (5)$$

where $|0\rangle, |1\rangle$ are eigenstates of the z component of the spin operator $\hat{S}_z = \frac{1}{2}\hat{\sigma}_z$ with eigenvalues $-\frac{1}{2}, \frac{1}{2}$ respectively. The corresponding density operator $\hat{\rho}_0 = |\psi_0\rangle\langle\psi_0|$ can be written in the form

$$\hat{\rho}_0 = \frac{1}{2}(\hat{I} + \mathbf{n} \cdot \boldsymbol{\sigma}), \quad (6)$$

where \hat{I} is the unity operator, $\mathbf{n} = (\sin(2\theta) \cos \varphi, \sin(2\theta) \sin \varphi, \cos(2\theta)) = \langle \boldsymbol{\sigma} \rangle$; $\boldsymbol{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ are the Pauli spin operators which in the matrix representation in the basis $|0\rangle, |1\rangle$ are

[†] In fact, in the case of pure states there always exists just one observable (at least in a sense of the Hermitian operator) such that the given pure state is an eigenstate of this observable. Unfortunately, it is impossible to specify this operator prior to complete reconstruction.

Table 1. In this table we present three observation levels $\mathcal{O}_A^{(1)}$; $\mathcal{O}_B^{(1)}$, and $\mathcal{O}_{\text{comp}}^{(1)}$ associated with a measurement of the particular spin- $\frac{1}{2}$ operators: (\bullet) , the observables that constitute a given observation level. We also present explicit expressions for the reconstructed density operators $\hat{\rho}_A$; $\hat{\rho}_B$ and ρ_{comp} .

Observation level	$\hat{\sigma}_z$	$\hat{\sigma}_x$	$\hat{\sigma}_y$	Reconstructed density operator
$\mathcal{O}_A^{(1)}$	•			$\hat{\rho}_A = \frac{1}{2}(\hat{I} + n_z \hat{\sigma}_z)$
$\mathcal{O}_B^{(1)}$	•	•		$\hat{\rho}_B = \frac{1}{2}(\hat{I} + n_z \hat{\sigma}_z + n_x \hat{\sigma}_x)$
$\mathcal{O}_{\text{comp}}^{(1)}$	•	•	•	$\hat{\rho}_{\text{comp}} = \frac{1}{2}(\hat{I} + n_z \hat{\sigma}_z + n_x \hat{\sigma}_x + n_y \hat{\sigma}_y)$

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{7}$$

To determine completely the unknown state, one has to measure three linearly independent (e.g. orthogonal) projections of the spin. After the measurement of the expectation value of each observable, a reconstruction of the generalized canonical density operator (3) according to the maximum-entropy principle can be performed. In table 1 we consider three observation levels defined as $\mathcal{O}_A^{(1)} = \{\hat{\sigma}_z\}$, $\mathcal{O}_B^{(1)} = \{\hat{\sigma}_z, \hat{\sigma}_x\}$ and $\mathcal{O}_C^{(1)} = \{\hat{\sigma}_z, \hat{\sigma}_x, \hat{\sigma}_y\} \equiv \mathcal{O}_{\text{comp}}$ (the superscript of the observation levels indicates the number of spins $\frac{1}{2}$ under consideration).

Using algebraic properties of the $\hat{\sigma}_\nu$ operators, the generalized canonical density operator (3) can be expressed as

$$\hat{\rho}^\sigma = \frac{1}{Z} \exp(-\lambda \cdot \sigma) = \frac{1}{Z} \left(\cosh |\lambda| \hat{I} - \sinh |\lambda| \frac{\lambda \cdot \sigma}{|\lambda|} \right), \quad Z = 2 \cosh |\lambda|, \tag{8}$$

with $\lambda = (\lambda_x, \lambda_y, \lambda_z)$ and $|\lambda|^2 = \lambda_x^2 + \lambda_y^2 + \lambda_z^2$. The final form of the $\hat{\rho}^\sigma$ on particular observation levels is given in table 1. The corresponding entropies can be written as

$$S_\sigma = p_\sigma \ln p_\sigma - (1 - p_\sigma) \ln (1 - p_\sigma), \tag{9}$$

where p_σ is one eigenvalue of $\hat{\rho}^\sigma$ (the other eigenvalue is equal to $1 - p_\sigma$) which reads as

$$p_A = \frac{1 + |\langle \hat{\sigma}_z \rangle|}{2}, \quad p_B = \frac{1 + ((\langle \hat{\sigma}_x \rangle)^2 + \langle \hat{\sigma}_z \rangle^2)^{1/2}}{2}, \quad p_{\text{comp}} = \frac{1 + ((\langle \hat{\sigma}_x \rangle)^2 + \langle \hat{\sigma}_y \rangle^2 + \langle \hat{\sigma}_z \rangle^2)^{1/2}}{2}. \tag{10}$$

It is seen that the entropy S_σ is equal to zero if and only if $p_\sigma = 1$. From here it follows that on $\mathcal{O}_A^{(1)}$ only the basis vectors $|0\rangle$ and $|1\rangle$ with $|\langle \hat{\sigma}_z \rangle| = 1$ can be fully reconstructed. $\mathcal{O}_B^{(1)}$, on which a whole set of pure states (5) with $\langle \hat{\sigma}_y \rangle = 0$ (i.e. $\varphi = 0, \pi$) can be uniquely determined, is non-trivial. For such states, $S_B = 0$, and further measurement of the $\hat{\sigma}_y$ on $\mathcal{O}_{\text{comp}}$ represents redundant (useless) information.

4. Two spins $\frac{1}{2}$

Now we assume a system composed of two *distinguishable* spins $\frac{1}{2}$. If we are performing only *local* measurements of observables such as $\hat{\sigma}_\mu^{(1)} \otimes \hat{I}^{(2)}$ and $\hat{I}^{(1)} \otimes \hat{\sigma}_\nu^{(2)}$ (here superscripts label the particles) which do not reflect correlations between the particles, then the reconstruction of the density operator reduces to an

estimation of individual (uncorrelated) spins $\frac{1}{2}$, that is the reconstruction reduces to the problem discussed in the previous section. For each spin $\frac{1}{2}$ the reconstruction can be performed separately and the resulting GCDO is given as a tensor product of particular generalized canonical density operators, that is $\hat{\rho} = \hat{\rho}^{(1)} \otimes \hat{\rho}^{(2)}$. In this case just the uncorrelated states $|\psi_0\rangle = |\psi_0^{(1)}\rangle \otimes |\psi_2^{(2)}\rangle$ can be fully reconstructed. Nevertheless, the correlated (non-factorable) states $|\psi_0\rangle \neq |\psi_0^{(1)}\rangle \otimes |\psi_2^{(2)}\rangle$ are of central interest.

In general, any density operator of a system composed of two distinguishable spins $\frac{1}{2}$ can be represented by a 4×4 Hermitian matrix and 15 independent numbers are required for its determination. It is worth noting that 15 operators (observables)

$$\{\hat{\sigma}_\mu^{(1)} \otimes \hat{I}^{(2)}, \hat{I}^{(1)} \otimes \hat{\sigma}_\nu^{(2)}, \hat{\sigma}_\mu^{(1)} \otimes \hat{\sigma}_\nu^{(2)}\} \quad (\mu, \nu = x, y, z) \quad (11)$$

together with the identity operator $\hat{I}^{(1)} \otimes \hat{I}^{(2)}$ form an operator algebra basis in which any operator can be expressed. In this ‘operator’ basis, each density operator can be written as

$$\hat{\rho} = \frac{1}{4} \left(\hat{I}^{(1)} \otimes \hat{I}^{(2)} + \mathbf{n}^{(1)} \cdot \boldsymbol{\sigma}^{(1)} \otimes \hat{I}^{(2)} + \mathbf{n}^{(2)} \cdot \hat{I}^{(1)} \otimes \boldsymbol{\sigma}^{(2)} + \sum_{\mu, \nu} \xi_{\mu\nu} \hat{\sigma}_\mu^{(1)} \otimes \hat{\sigma}_\nu^{(2)} \right) \quad (12)$$

with $\xi_{\mu\nu} = \langle \hat{\sigma}_\mu^{(1)} \otimes \hat{\sigma}_\nu^{(2)} \rangle$ ($\mu, \nu = x, y, z$).

Using the maximum-entropy principle we can (partially) reconstruct an unknown density operator $\hat{\rho}_0$ on various observation levels. Conceptually the method of maximum entropy is rather straightforward; one has to express the generalized canonical density operator (3) for two spins $\frac{1}{2}$ in the form (12) from which a set of nonlinear equations for Lagrange multipliers λ_ν is obtained. Owing to algebraic properties of the operators under consideration the practical realization of this programme can be technically difficult (see appendix A).

In table 2 we define some non-trivial observation levels. Measured observables which define a particular observation level are indicated in table 2 by full circles while the open circles indicate unmeasured observables (i.e. these observables are not included in the given observation level) for which the maximum-entropy principle ‘predicts’ non-zero mean values. This means that the maximum-entropy principle provides us with a non-trivial estimation of mean values of unmeasured observables. The generalized canonical density operators which correspond to the observation levels considered in table 2 are presented in table 3. The signs \oplus and \ominus are used to indicate unmeasured observables for which non-trivial information can be obtained with the help of the maximum-entropy principle.

4.1. Reconstruction of Bell states

In what follows we analyse a partial reconstruction of the Bell states (i.e. the most correlated two particle states) on observation levels given in table 2. One of our main tasks will be to find the minimum observation level (i.e. the set of system observables) on which the complete reconstruction of these states can be performed. Obviously, if all 15 observables are measured, then any state of two spins $\frac{1}{2}$ can be reconstructed precisely. Nevertheless, owing to the quantum entanglement between the two particles, measurements of some observables will simply be redundant. To find the minimal set of observables which uniquely determine the Bell state one has to perform either a sequence of reductions of the complete

Table 3. We present explicit expressions for the reconstructed density operators $\hat{\rho}$ of two spins $\frac{1}{2}$ on the observation levels denoted in table 2. We use the notation $n_\mu^{(p)} = \langle \hat{\sigma}_\mu^{(p)} \rangle$ ($\mu = x, y, z$; $p = 1, 2$) and $\xi_{\mu\nu} = \langle \hat{\sigma}_\mu^{(1)} \hat{\sigma}_\nu^{(2)} \rangle$ with $\mu, \nu = x, y, z$. The signs \oplus and \ominus are used to indicate unmeasured observables for which non-trivial information can be obtained with the help of the maximum-entropy principle.

Observation level	Reconstructed density operator
$\mathcal{O}_A^{(2)}$	$\hat{\rho}_A = \frac{1}{4} I^{(1)} I^{(2)} + n_z^{(1)} \hat{\sigma}_z^{(1)} I^{(2)} + n_z^{(2)} I^{(1)} \hat{\sigma}_z^{(2)} \oplus n_z^{(1)} n_z^{(2)} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} = \frac{1}{4} (I^{(1)} + n_z^{(1)} \hat{\sigma}_z^{(1)}) (I^{(2)} + n_z^{(2)} \hat{\sigma}_z^{(2)})$
$\mathcal{O}_B^{(2)}$	$\hat{\rho}_B = \frac{1}{4} I^{(1)} I^{(2)} + n_z^{(1)} \hat{\sigma}_z^{(1)} I^{(2)} + n_z^{(2)} I^{(1)} \hat{\sigma}_z^{(2)} + \xi_{xz} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)}$
$\mathcal{O}_C^{(2)}$	$\hat{\rho}_C = \frac{1}{4} I^{(1)} I^{(2)} + n_z^{(1)} \hat{\sigma}_z^{(1)} I^{(2)} + n_z^{(2)} I^{(1)} \hat{\sigma}_z^{(2)} + \xi_{yz} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} + \xi_{zx} \hat{\sigma}_z^{(1)} \hat{\sigma}_x^{(2)}$
$\mathcal{O}_D^{(2)}$	$\hat{\rho}_D = \frac{1}{4} I^{(1)} I^{(2)} + n_z^{(1)} \hat{\sigma}_z^{(1)} I^{(2)} + n_z^{(2)} I^{(1)} \hat{\sigma}_z^{(2)} + n_x^{(2)} I^{(1)} \hat{\sigma}_x^{(2)} + \xi_{yz} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} + \xi_{zx} \hat{\sigma}_z^{(1)} \hat{\sigma}_x^{(2)} + \xi_{xy} \hat{\sigma}_z^{(1)} \hat{\sigma}_y^{(2)} + \xi_{xx} \hat{\sigma}_z^{(1)} \hat{\sigma}_x^{(2)} + \xi_{yy} \hat{\sigma}_z^{(1)} \hat{\sigma}_y^{(2)}$
$\mathcal{O}_E^{(2)}$	$\hat{\rho}_E = \frac{1}{4} I^{(1)} I^{(2)} + \xi_{zz} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} + \xi_{xx} \hat{\sigma}_x^{(1)} \hat{\sigma}_x^{(2)} \ominus \xi_{zz} \xi_{xx} \hat{\sigma}_y^{(1)} \hat{\sigma}_y^{(2)}$
$\mathcal{O}_F^{(2)}$	$\hat{\rho}_F = \frac{1}{4} I^{(1)} I^{(2)} + \xi_{zz} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} + \xi_{xx} \hat{\sigma}_x^{(1)} \hat{\sigma}_x^{(2)} + \xi_{yy} \hat{\sigma}_y^{(1)} \hat{\sigma}_y^{(2)}$
$\mathcal{O}_G^{(2)}$	$\hat{\rho}_G = \frac{1}{4} I^{(1)} I^{(2)} + \xi_{zz} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} + \xi_{xx} \hat{\sigma}_x^{(1)} \hat{\sigma}_x^{(2)} + \xi_{yy} \hat{\sigma}_y^{(1)} \hat{\sigma}_y^{(2)} + \xi_{yx} \hat{\sigma}_x^{(1)} \hat{\sigma}_y^{(2)} + \xi_{xy} \hat{\sigma}_y^{(1)} \hat{\sigma}_x^{(2)} + \xi_{xx} \hat{\sigma}_x^{(1)} \hat{\sigma}_x^{(2)}$
$\mathcal{O}_H^{(2)}$	$\hat{\rho}_H = \frac{1}{4} I^{(1)} I^{(2)} + \xi_{xx} \hat{\sigma}_x^{(1)} \hat{\sigma}_x^{(2)} + \xi_{yy} \hat{\sigma}_y^{(1)} \hat{\sigma}_y^{(2)} + \xi_{yx} \hat{\sigma}_x^{(1)} \hat{\sigma}_y^{(2)} + \xi_{xy} \hat{\sigma}_y^{(1)} \hat{\sigma}_x^{(2)} \oplus I \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)}; \quad I = \xi_{xy} \xi_{yx} - \xi_{xx} \xi_{yy}$
$\mathcal{O}_I^{(2)}$	$\hat{\rho}_I = \frac{1}{4} I^{(1)} I^{(2)} + n_z^{(1)} \hat{\sigma}_z^{(1)} I^{(2)} + n_x^{(2)} I^{(1)} \hat{\sigma}_x^{(2)} + \xi_{zz} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} + \xi_{xx} \hat{\sigma}_x^{(1)} \hat{\sigma}_x^{(2)} \oplus n_z^{(1)} n_x^{(2)} \hat{\sigma}_z^{(1)} \hat{\sigma}_x^{(2)} \oplus \theta \hat{\sigma}_x^{(1)} \hat{\sigma}_y^{(2)}$
$\mathcal{O}_J^{(2)}$	$\hat{\rho}_J = \frac{1}{4} I^{(1)} I^{(2)} + n_z^{(1)} \hat{\sigma}_z^{(1)} I^{(2)} + n_x^{(2)} I^{(1)} \hat{\sigma}_x^{(2)} + \xi_{zz} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} + \xi_{xx} \hat{\sigma}_x^{(1)} \hat{\sigma}_x^{(2)} + \xi_{yy} \hat{\sigma}_y^{(1)} \hat{\sigma}_y^{(2)} \oplus u \hat{\sigma}_z^{(1)} \hat{\sigma}_x^{(2)} \oplus v \hat{\sigma}_x^{(1)} \hat{\sigma}_z^{(2)} \oplus w \hat{\sigma}_y^{(1)} \hat{\sigma}_y^{(2)}$

observation level, or a systematic extension of the most trivial observation level $\mathcal{O}_A^{(2)}$.

Let us consider particular examples of Bell states, of the form

$$|\psi_{\varphi}^{(\text{Bell})}\rangle = \frac{1}{2^{1/2}}[|1, 1\rangle + \exp(i\varphi)|0, 0\rangle], \hat{\rho}_{\varphi}^{(\text{Bell})} = |\psi_{\varphi}^{(\text{Bell})}\rangle\langle\psi_{\varphi}^{(\text{Bell})}| \tag{13}$$

(other Bell states are discussed later). These maximally correlated states have the property that the result of a measurement performed on one of the two spins $\frac{1}{2}$ uniquely determines the state of the second spin. Therefore, these states find their applications in quantum communication systems [18]. In addition, they are suitable for testing fundamental principles of quantum mechanics [19] such as the complementarity principle or local hidden-variable theories [20].

Let us analyse now a sequence of successive extensions of the observation level $\mathcal{O}_A^{(2)}$:

$$\mathcal{O}_A^{(2)} \subset \mathcal{O}_B^{(2)} \subset \mathcal{O}_C^{(2)} \subset \mathcal{O}_D^{(2)}. \tag{14}$$

The observation level $\mathcal{O}_A^{(2)}$ (see table 2) is associated with the measurement of $\hat{\sigma}_z$ observables of each spin individually, that is it is insensitive with respect to correlations between the spins. On $\mathcal{O}_B^{(2)}$ both z -spin components of particular spins and their correlation have been recorded (simultaneous measurement of these observables is possible because they commute). Further extension to the observation level on $\mathcal{O}_C^{(2)}$ corresponds to a rotation of the Stern–Gerlach apparatus such that the x -spin component of the second spin $\frac{1}{2}$ is measured. The observation level $\mathcal{O}_D^{(2)}$ is associated with another rotation of the Stern–Gerlach apparatus which would allow us to measure the y -spin component. The generalized canonical density operators on the observation levels $\mathcal{O}_B^{(2)}$, $\mathcal{O}_C^{(2)}$ and $\mathcal{O}_D^{(2)}$ predict zero mean values for all the unmeasured observables (11) (see table 3).

In general, successive extensions (14) of the observation level $\mathcal{O}_A^{(2)}$ should be accompanied by a decrease in the entropy of the reconstructed state which should reflect an increase in our knowledge about the quantum-mechanical system under consideration. Nevertheless, we note that there are states for which the entropy remains constant when $\mathcal{O}_B^{(2)}$ is extended towards $\mathcal{O}_C^{(2)}$ and $\mathcal{O}_D^{(2)}$, that is the measurements performed are in fact redundant. For instance, this is the case for the maximally correlated state (13). Here entropies associated with given observation levels are

$$S_A = 2 \ln 2, \quad S_B = S_C = S_D = \ln 2, \tag{15}$$

respectively, which mean that these observation levels are not suitable for reconstruction of the Bell states. The reason is that the Bell states have no ‘preferential’ direction for each individual spin, that is $\langle \hat{\sigma}_{\mu}^{(p)} \rangle = 0$ for $\mu = x, y, z$ and $p = 1, 2$.

From the above it follows that, for a non-trivial reconstruction of Bell states, the observables which reflect correlations between composite spins also have to be included into the observation level. Therefore let us now discuss the sequence of observation levels

$$\mathcal{O}_E^{(2)} \subset \mathcal{O}_F^{(2)} \subset \mathcal{O}_G^{(2)} \tag{16}$$

associated with simultaneous measurement of spin components of the two particles (see table 2). The corresponding GCDOs are given in table 3. To answer the

question of which states can be completely reconstructed on the observation level $\mathcal{O}_E^{(2)}$ we evaluate the von Neumann entropy (2) of the GCDO $\hat{\rho}_E$. For the Bell states we find that $S_E = -p_E \ln p_E - (1 - p_E) \ln (1 - p_E)$ where $p_E = (1 - \cos \varphi)/2$. We can also compare directly $\hat{\rho}_\varphi^{(\text{Bell})}$ with $\hat{\rho}_E$. The density operator $\hat{\rho}_\varphi^{(\text{Bell})}$ in the matrix form can be written as

$$\hat{\rho}_\varphi^{(\text{Bell})} = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & \exp(-i\varphi) \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \exp(i\varphi) & 0 & 0 & 1 \end{bmatrix}, \quad (17)$$

while the corresponding operator reconstructed on the observation level $\mathcal{O}_E^{(2)}$ is

$$\hat{\rho}_E = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & \cos \varphi \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \cos \varphi & 0 & 0 & 1 \end{bmatrix}. \quad (18)$$

We see that $\hat{\rho}_\varphi^{(\text{Bell})} = \hat{\rho}_E$ and $S[\hat{\rho}_E] = 0$ only if $\varphi = 0$ or π which means that the Bell states $|\Psi_{\varphi=0,\pi}\rangle = (1/2^{1/2})[|1,1\rangle \pm |0,0\rangle]$ are completely determined by mean values of two observables $\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)}$ and $\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)}$ and that these states can be completely reconstructed on \mathcal{O}_E . We note that two other maximally correlated states $|\Phi \pm\rangle = (1/2^{1/2})[|0,1\rangle \pm |1,0\rangle]$ can also be completely reconstructed on $\mathcal{O}_E^{(2)}$.

The extension of $\mathcal{O}_E^{(2)}$ to $\mathcal{O}_F^{(2)}$ does not increase the amount of information about the Bell states (13) with $\varphi \neq 0, \pi$. For this reason we have to consider further extension of $\mathcal{O}_F^{(2)}$ to the observation level $\mathcal{O}_G^{(2)}$ (see table 2 and appendix A). In what follows we shall show that this is an observation level on which *all* Bell states (13) can be completely reconstructed. To see this, one has to realize two facts. Firstly, the GCDO $\hat{\rho}_G$ given by equation (3) can be expressed as a linear superposition of observables associated with the given observation level, that is

$$\begin{aligned} \hat{\rho}_G &= \frac{1}{Z_G} \exp \left(- \sum_{\mu=x,y,z} \lambda_{\mu\mu} \hat{\sigma}_\mu^{(1)} \otimes \hat{\sigma}_\mu^{(2)} - \lambda_{xy} \hat{\sigma}_x^{(1)} \otimes \sigma_y^{(2)} - \lambda_{yx} \sigma_y^{(1)} \otimes \hat{\sigma}_x^{(2)} \right) \\ &= \frac{1}{4} \left(\hat{1} - \sum_{\mu=x,y,z} \xi_{\mu\mu} \hat{\sigma}_\mu^{(1)} \otimes \hat{\sigma}_\mu^{(2)} - \xi_{xy} \hat{\sigma}_x^{(1)} \otimes \sigma_y^{(2)} - \xi_{yx} \sigma_y^{(1)} \otimes \hat{\sigma}_x^{(2)} \right) \end{aligned} \quad (19)$$

where the parameters $\xi_{\mu\nu}$ are functions of the Lagrange multipliers $\lambda_{\mu\nu}$. Secondly, for Bell states (13) the only observables which have non-zero expectation values are those associated with $\mathcal{O}_G^{(2)}$, namely $\langle \hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} \rangle = 1$, $\langle \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)} \rangle = -\langle \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)} \rangle = \cos \varphi$ and $\langle \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_y^{(2)} \rangle = \langle \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_x^{(2)} \rangle = \sin \varphi$. This means that all coefficients in the GCDO $\hat{\rho}_G$ given by equation (12) are uniquely determined by the measurement, that is $\hat{\rho}_G = \hat{\rho}_\varphi^{(\text{Bell})}$.

From the above it follows that Bell states can be completely reconstructed on the observation level $\mathcal{O}_G^{(2)}$. On the other hand, $\mathcal{O}_G^{(2)}$ is not the *minimum* observation level on which these states can be completely reconstructed. The minimum set of observables which would allow us to reconstruct Bell states uniquely can be found by a *reduction* in $\mathcal{O}_G^{(2)}$. Direct inspection of a finite number of possible reductions

reveals that Bell states can be completely reconstructed on those observation levels which can be obtained from $\mathcal{O}_G^{(2)}$ when one of the observables $\hat{\sigma}_\nu^{(1)} \otimes \hat{\sigma}_\nu^{(2)}$ ($\nu = x, y, z$) is omitted. As an example, let us consider the observation level \mathcal{O}_H given in table 2 which represents a reduction in $\mathcal{O}_G^{(2)}$ when the observable $\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)}$ is omitted. Performing the Taylor series expansion of the generalized canonical density operator $\hat{\rho}_H$ defined by equation (3), one can find that the only new observable $\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)}$ enters the expression for the $\hat{\rho}_H$ as indicated in table 3. The coefficient t in front of $\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)}$ either can be found explicitly in a closed analytical form (see appendix A) or can be obtained from the following variational problem. That is, we remind ourselves that equation (3) for $\hat{\rho}_H$ helps us to identify those unmeasured observables for which the Jaynes principle of the maximum entropy ‘predicts’ non-zero mean values. At this stage we still have to find the particular value of the parameter t for which the density operator $\hat{\rho}_H$ in table 3 leads to the maximum of the von Neumann entropy. To do so we search through the one-dimensional parametric space which is bounded as $-1 \leq t \leq 1$. To be specific, first of all, for $t \in (-1, 1)$ we have to exclude those operators which are not true density operators (i.e. any such operators which have negative eigenvalues). Then we ‘pick’ up from a physical parametric subspace the GCDO with the maximum von Neumann entropy. Direct calculation for Bell states shows that the physical parametric subspace is reduced to an isolated ‘point’ with $t = \langle \hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} \rangle = 1$. Therefore we conclude that Bell states can be completely reconstructed on \mathcal{O}_H . Two other minimum observation levels suitable for the complete reconstruction of Bell states can be obtained by a reduction in $\mathcal{O}_G^{(2)}$ when either $\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)}$ or $\hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)}$ is omitted. On the other hand, direct inspection shows that a reduction in $\mathcal{O}_G^{(2)}$ by exclusion of either $\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_y^{(2)}$ or $\hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_z^{(2)}$ leads to an incomplete observation level with respect to Bell states.

In what follows we discuss briefly two other observation levels $\mathcal{O}_I^{(2)}$ and $\mathcal{O}_J^{(2)}$ which are defined in table 2. The observation level $\mathcal{O}_I^{(2)}$ serves as an example when one can find an analytical expression for the Taylor series expansion of the canonical density operator $\hat{\rho}_I$ (equation (3)) in the form (12). The coefficients (functions of the original Lagrange multipliers) in front of particular observables in equation (12) can be identified and are given in table 3. Problems do appear when $\mathcal{O}_I^{(2)}$ is extended towards $\mathcal{O}_J^{(2)}$. In this case we cannot simplify the exponential expression (3) for $\hat{\rho}_I$ and rewrite it analytically in the form (12) as a linear combination of the observables (11). In this situation, one should apply the following procedure: firstly, by performing the Taylor series expansion of $\hat{\rho}_I$ to the lowest orders, one can identify the observables with non-zero coefficients in the form (12). That is, for $\hat{\rho}_I$ the additional observables $\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_x^{(2)}$, $\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_z^{(2)}$ and $\hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)}$ appear in addition to those which form $\mathcal{O}_J^{(2)}$ (see table 3). The corresponding coefficients $u, v, w \in (-1, 1)$ form a bounded three-dimensional parametric space (u, v, w) . In the second step, one can use constructively the maximum-entropy principle to choose within this parametric space the density operator with the maximum von Neumann entropy. The basic procedure is to scan the whole three-dimensional parametric space. At the beginning, one has to select out those density operators (i.e. those parameters u, v, w) which possess negative eigenvalues and do not represent genuine density operators. Finally, from a remaining set of ‘physical’ density operators which are semipositively defined the canonical density operator $\hat{\rho}_I$ with maximum von Neumann entropy has to be

chosen. For completeness, let us note that for Bell states the observation levels $\mathcal{O}_I^{(2)}$ and $\mathcal{O}_J^{(2)}$ are equivalent to $\mathcal{O}_E^{(2)}$, that is, $\hat{\rho}_I = \hat{\rho}_J = \hat{\rho}_E$.

In this section we have found the minimum observation levels (e.g. $\mathcal{O}_H^{(2)}$) which are suitable for the complete reconstruction of Bell states. These observation levels are associated with the measurement of two-spin correlations $\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_z^{(2)}$, $\hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_z^{(2)}$ and two of the observables $\hat{\sigma}_\nu^{(1)} \otimes \hat{\sigma}_\nu^{(2)}$ ($\nu = x, y, z$). Once this problem has been solved, it is interesting then to find a minimum set of observables suitable for a complete reconstruction of maximally correlated states of systems consisting of more than two spins $\frac{1}{2}$. In the following section we shall investigate the (partial) reconstruction of GHZ states of three spins $\frac{1}{2}$ on various observation levels.

5. Three spins $\frac{1}{2}$

Even though the Jaynes principle of maximum entropy provides us with general instructions on how to reconstruct density operators of quantum-mechanical systems, practical applications of this reconstruction scheme may face serious difficulties. In many cases the reconstruction scheme fails because of insurmountable technical problems (e.g. the system of equations for Lagrange multipliers cannot be solved explicitly). We have illustrated these problems in the previous section when we have discussed the reconstruction of a density operator of two spins $\frac{1}{2}$. Obviously, the general problem of reconstruction of density operators describing a system composed of three spins $\frac{1}{2}$ is much more difficult. Nevertheless a (partial) reconstruction of some states of this system can be performed. In particular, in this section we shall discuss a reconstruction of the maximally correlated three spin $\frac{1}{2}$ states, the so-called GHZ states [20]:

$$|\Psi_\varphi^{(\text{GHZ})}\rangle \frac{1}{2^{1/2}} [|1, 1, 1\rangle + \exp(i\varphi)|0, 0, 0\rangle], \quad \hat{\rho}_\varphi^{(\text{GHZ})} = |\Psi_\varphi\rangle\langle\Psi_\varphi|. \quad (20)$$

Our main task will be to identify, with the help of the Jaynes principle of maximum entropy, the minimum observation level on which the GHZ state can be completely reconstructed.

We start with a relatively simple observation level $\mathcal{O}_B^{(3)}$ such that only *two*-particle correlations of the neighbouring spins are measured, that is

$$\mathcal{O}_B^{(3)} = \{\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{I}^{(3)}, \hat{I}^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{\sigma}_z^{(3)}\}. \quad (21)$$

The generalized density operator associated with this observation level is

$$\begin{aligned} \hat{\rho}_B = & \frac{1}{8} [\hat{I}^{(1)} \otimes \hat{I}^{(2)} \otimes \hat{I}^{(3)} + \langle \hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{I}^{(3)} \rangle \hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{I}^{(3)} \\ & + \langle \hat{I}^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{\sigma}_z^{(3)} \rangle \hat{I}^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{\sigma}_z^{(3)} \\ & \oplus \langle \hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{I}^{(3)} \rangle \hat{I}^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{\sigma}_z^{(3)} \hat{\sigma}_z^{(1)} \otimes \hat{I}^{(2)} \otimes \hat{\sigma}_z^{(3)}], \end{aligned} \quad (22)$$

where \oplus indicates a prediction for the unmeasured observable. In particular, for the GHZ states (20) we obtain the following GCDO:

$$\begin{aligned} \hat{\rho}_B^{(\text{GHZ})} = & \frac{1}{8} [\hat{I}^{(1)} \otimes \hat{I}^{(2)} \otimes \hat{I}^{(3)} \\ & + \hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{I}^{(3)} + \hat{I}^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{\sigma}_z^{(3)} \oplus \hat{\sigma}_z^{(1)} \otimes \hat{I}^{(2)} \otimes \hat{\sigma}_z^{(3)}] \\ = & \frac{1}{2} |1, 1, 1\rangle\langle 1, 1, 1| + \frac{1}{2} |0, 0, 0\rangle\langle 0, 0, 0|. \end{aligned} \quad (23)$$

The reconstructed density operator $\hat{\rho}_B^{(\text{GHZ})}$ describes a mixture of three-particle states and it does not contain any information about the three-particle correlations associated with the GHZ states. In other words, on $\mathcal{O}_B^{(3)}$ the phase information which plays an essential role in the description of quantum entanglement cannot be reconstructed. This is because the density operator $\hat{\rho}_B^{(\text{GHZ})}$ is equal to the phase-averaged GHZ density operator, that is

$$\hat{\rho}_B^{(\text{GHZ})} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{\rho}_{\varphi}^{(\text{GHZ})} d\varphi. \quad (24)$$

Because of this loss of information, the von Neumann entropy of the state $\hat{\rho}_B^{(\text{GHZ})}$ is equal to $\ln 2$. We note that, when the GHZ states are reconstructed on the observation levels $\mathcal{O}_{B'}^{(3)} = \{\hat{\sigma}_{\mu}^{(1)} \otimes \hat{\sigma}_{\mu}^{(2)} \otimes \hat{I}^{(3)}, \hat{I}^{(1)} \otimes \hat{\sigma}_{\mu}^{(2)} \otimes \hat{\sigma}_{\mu}^{(3)}\}$ ($\mu = x, y$), then the corresponding reconstructed operators are again given by equation (23). These examples illustrate the fact that three-particle correlation cannot in general be reconstructed via the measurement of two-particle correlations.

To find the observation level on which the complete reconstruction of the GHZ states can be performed, we recall the observables which may have non-zero mean values for these states. Using the abbreviations

$$\begin{aligned} \xi_{\mu\nu} &= \langle \hat{\sigma}_{\mu}^{(1)} \otimes \hat{\sigma}_{\nu}^{(2)} \otimes \hat{I}^{(3)} \rangle, \quad \xi_{\mu\nu\omega} = \langle \hat{I}^{(1)} \otimes \hat{\sigma}_{\mu}^{(2)} \otimes \hat{\sigma}_{\nu}^{(3)} \rangle, \quad \xi_{\mu\nu\omega} = \langle \hat{\sigma}_{\mu}^{(1)} \otimes \hat{I}^{(2)} \otimes \hat{\sigma}_{\nu}^{(3)} \rangle, \\ \zeta_{\mu\nu\omega} &= \langle \hat{\sigma}_{\mu}^{(1)} \otimes \hat{\sigma}_{\nu}^{(2)} \otimes \hat{\sigma}_{\omega}^{(3)} \rangle, \quad (\mu, \nu, \omega = x, y, z), \end{aligned} \quad (25)$$

we find the non-zero mean values to be

$$\begin{aligned} \xi_{z_1 z_2} &= \xi_{z_2 z_3} = \xi_{z_1 z_3} = 1, \\ \zeta_{x_1 x_2 y_3} &= \zeta_{y_1 x_2 x_3} = \zeta_{x_1 y_2 x_3} = \sin \varphi, \\ \zeta_{y_1 y_2 y_3} &= \zeta_{x_1 y_2 y_3} = \zeta_{y_1 x_2 y_3} = -\cos \varphi \\ \zeta_{x_1 x_2 x_3} &= \cos \varphi, \\ \zeta_{y_1 y_2 y_3} &= -\sin \varphi. \end{aligned} \quad (26)$$

We see that for arbitrary φ there exist non-vanishing three-particle correlations $\zeta_{\mu\nu\omega}$. The observation level which consists of all the observables with non-zero mean values is the complete observation level with respect to the GHZ states. Our task now is to reduce this set of observables to a minimum observation level on which the GHZ states can still be uniquely determined. In practice it means that each observation level which is suitable for the detection of the existing coherence and correlations should incorporate some of the observables with non-zero mean values. The other observables of these observation levels should result as a consequence of mutual tensor products which appear in the Taylor series expansion of the GCDO (3). It can be seen by direct inspection of the finite number of possible reductions that the minimum set of the observables which matches these requirements consists of two two-spin observables and two three-spin observables. For the illustration we consider the observation level

$$\mathcal{O}_C^{(3)} = \{\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{I}^{(3)}, \hat{I}^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{\sigma}_z^{(3)}, \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)} \otimes \hat{\sigma}_x^{(3)}, \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)} \otimes \hat{\sigma}_y^{(3)}\}. \quad (27)$$

In this case the exponent \hat{C} of the GCDO $\hat{\rho}_C = \exp(-\hat{C})/Z_C$ (see equation (3)) can be rewritten as $\hat{C} = \hat{C}_1 + \hat{C}_2$ with $\hat{C}_1 = \gamma_{12}\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(1)} \otimes \hat{I}^{(3)} + \gamma_{23}\hat{I}^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{\sigma}_z^{(3)}$ and $\hat{C}_2 = \alpha\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)} \otimes \hat{\sigma}_x^{(3)} + \beta\hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)} \otimes \hat{\sigma}_y^{(3)}$. The operators \hat{C}_1, \hat{C}_2 commute and further calculations are straightforward. After some algebra the GCDO $\hat{\rho}_C$ can be found in the form

$$\begin{aligned} \hat{\rho}_C = & \frac{1}{8}[\hat{I}^{(1)} \otimes \hat{I}^{(2)} \otimes \hat{I}^{(3)} + \xi_{z_1 z_2} \hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{I}^{(3)} + \xi_{z_2 z_3} \hat{I}^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{\sigma}_z^{(3)} \\ & + \zeta_{x_1 x_2 x_3} \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)} \otimes \hat{\sigma}_x^{(3)} + \zeta_{y_1 y_2 y_3} \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)} \otimes \hat{\sigma}_y^{(3)} \oplus \xi_{z_1 z_2} \xi_{z_2 z_3} \hat{\sigma}_z^{(1)} \otimes \hat{I}^{(2)} \otimes \hat{\sigma}_z^{(3)} \\ & \ominus \zeta_{x_1 x_2 x_3} (\xi_{z_1 z_2} \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)} \otimes \hat{\sigma}_x^{(3)} + \xi_{z_2 z_3} \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_y^{(2)} \otimes \hat{\sigma}_y^{(3)} \\ & + \xi_{z_1 z_2} \xi_{z_2 z_3} \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_x^{(2)} \otimes \hat{\sigma}_y^{(3)}) \ominus \zeta_{y_1 y_2 y_3} (\xi_{z_1 z_2} \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)} \otimes \hat{\sigma}_y^{(3)} \\ & + \xi_{z_2 z_3} \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_x^{(2)} \otimes \hat{\sigma}_x^{(3)} + \xi_{z_1 z_2} \xi_{z_2 z_3} \hat{\sigma}_{yx}^{(1)} \otimes \hat{\sigma}_y^{(2)} \otimes \hat{\sigma}_x^{(3)})]. \end{aligned} \quad (28)$$

For the GHZ states the von Neumann entropy of the GCDO $\hat{\rho}_C$ is equal to zero, from which it follows that $\hat{\rho}_C = \hat{\rho}_\varphi^{(\text{GHZ})}$ (see equation (20)), that is the GHZ states can be completely reconstructed on $\mathcal{O}_C^{(3)}$. Moreover, the observation level \mathcal{O}_C represents the *minimum* set of observables for complete determination of the GHZ states.

6. Conclusions

We have investigated the problem of a (partial) reconstruction of correlated spin states on different observation levels. We have found the minimal set of observables for the complete reconstruction of the most correlated states for systems composed of two and three spins $\frac{1}{2}$, that is Bell states and GHZ states. Direct generalization to systems of more spins $\frac{1}{2}$ is possible.

The concept of observation levels and the maximum-entropy principle is a powerful tool which can be used also for other physical systems, for example for the reconstruction of the states of a monochromatic light field [21]. We recall that this reconstruction scheme is based on the knowledge of the *exact* mean values of given observables or their probability distributions (see appendix A). Theoretically, this means that an *infinite* number of measurements over an ensemble of identically prepared systems have to be performed in order to obtain those mean values which are needed. In practice, if the number of measurements is sufficiently high, then the mean values can be considered to be measured precisely enough and the Jaynes principle can be applied for a state reconstruction. On the other hand, if just a few measurements are performed, then the mean values of the considered observables are not known and the Jaynes principle cannot be used.

In this case another reconstruction scheme has to be applied. In particular, in the case of a small number of measurements the Bayesian reconstruction scheme [22] can be effectively utilized. We shall address the problem of a reconstruction of correlated spin systems based on Bayesian methods elsewhere [23].

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Appendix A

Conceptually the reconstruction scheme based on the Jaynes principle of the maximum entropy is very simple. On the other hand, particular analytical calculations can be difficult and in many cases cannot be performed. In this appendix we present explicit calculations of GCDOs and corresponding entropies for two observation levels $\mathcal{O}_G^{(2)}$ and $\mathcal{O}_H^{(2)}$ defined in table 2.

A.1. Observation level $\mathcal{O}_G^{(2)}$

Let us assume the observation level $\mathcal{O}_G^{(2)}$ given by the set of observables $\{\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)}; \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)}; \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_y^{(2)}; \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_x^{(2)}; \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)}\}$. In this case the GCDO is

$$\hat{\rho}_G = \frac{1}{Z_G} \exp(-\hat{E}), \quad (\text{A } 1)$$

where

$$Z_G = \text{Tr}[\exp(-\hat{E})] \quad (\text{A } 2)$$

is the partition function. Here we have used the abbreviation

$$\hat{E} = \lambda_{zz} \hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} + \lambda_{xx} \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)} + \lambda_{xy} \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_y^{(2)} + \lambda_{yx} \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_x^{(2)} + \lambda_{yy} \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)}. \quad (\text{A } 3)$$

The corresponding entropy has the form

$$S_G = \ln Z_G + \lambda_{zz} \xi_{zz} + \lambda_{xx} \xi_{xx} + \lambda_{xy} \xi_{xy} + \lambda_{yx} \xi_{yx} + \lambda_{yy} \xi_{yy}, \quad (\text{A } 4)$$

Using the algebraic properties of the operators associated with the given observation level we find that the GCDO (A 1) is

$$\begin{aligned} \hat{\rho}_G = & \frac{1}{4} [\hat{I}^{(1)} \otimes \hat{I}^{(2)} + \xi_{zz} \hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} + \xi_{xx} \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)} \\ & + \xi_{xy} \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_y^{(2)} + \xi_{yx} \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_x^{(2)} + \xi_{yy} \hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)}], \end{aligned} \quad (\text{A } 5)$$

where we use the notation

$$\xi_{\mu\nu} \equiv \langle \hat{\sigma}_\mu^{(1)} \otimes \hat{\sigma}_\nu^{(2)} \rangle \quad (\mu, \nu = x, y, z). \quad (\text{A } 6)$$

Now we express the entropy as a function of expectation values of operators associated with the observation level $\mathcal{O}_G^{(2)}$. With the help of this entropy function we can perform reductions in $\mathcal{O}_G^{(2)}$ to the observation levels $\mathcal{O}_H^{(2)}$, $\mathcal{O}_F^{(2)}$ and $\mathcal{O}_E^{(2)}$. In order to perform this reduction we express $\lambda_{\mu\nu}$ in equation (A 4) as functions of the expectation values $\xi_{\mu\nu}$. To do so we utilize the relation

$$\xi_{\mu\nu} = \frac{\partial(\ln Z_G)}{\partial \lambda_{\mu\nu}}. \quad (\text{A } 7)$$

The partition function Z_G can be found when we rewrite the operator \hat{E} in equation (A 4) as a 4×4 matrix:

$$\hat{E} = \begin{bmatrix} a & 0 & 0 & d^* \\ 0 & -a & b^* & 0 \\ 0 & b & -a & 0 \\ d & 0 & 0 & a \end{bmatrix}, \quad (\text{A } 8)$$

where we used the abbreviations

$$a = \lambda_{zz}, \quad b = \lambda_{xx} + \lambda_{yy} - i(\lambda_{xy} - \lambda_{yx}), \quad d = \lambda_{xx} - \lambda_{yy} + i(\lambda_{xy} + \lambda_{yx}). \quad (\text{A } 9)$$

The powers of the operator \hat{E} can be written as

$$\hat{E}^n = \begin{bmatrix} E_{11}^{(n)} & 0 & 0 & E_{14}^{(n)} \\ 0 & E_{22}^{(n)} & E_{23}^{(n)} & 0 \\ 0 & E_{32}^{(n)} & E_{33}^{(n)} & 0 \\ E_{41}^{(n)} & 0 & 0 & E_{44}^{(n)} \end{bmatrix}. \quad (\text{A } 10)$$

with the matrix elements given by the relations

$$\begin{aligned} E_{11}^{(n)} &= E_{44}^{(n)} = \frac{1}{2}[(a + |d|)^n + (a - |d|)^n], \\ E_{14}^{(n)} &= \frac{1}{2}[(a + |d|)^n - (a - |d|)^n] \frac{d^*}{|d|}, \\ E_{22}^{(n)} &= E_{33}^{(n)} = \frac{1}{2}(-a + |b|)^n + (-a - |b|)^n, \\ E_{23}^{(n)} &= \frac{1}{2}(-a + |b|)^n - (-a - |b|)^n \frac{b^*}{|b|}, \\ E_{32}^{(n)} &= E_{23}^{(n)*}, \\ E_{41}^{(n)} &= E_{14}^{(n)*}. \end{aligned} \quad (\text{A } 11)$$

Now we find that

$$\exp(-\hat{E}) = \begin{bmatrix} \exp(-a) \cosh |d| & 0 & 0 & -\exp(-a) \sinh(|d|) \frac{d^*}{|d|} \\ 0 & \exp a \cosh |b| & -\exp a \sinh(|b|) \frac{b^*}{|b|} & 0 \\ 0 & -\exp a \sinh(|b|) \frac{b}{|b|} & \exp a \cosh |b| & 0 \\ -\exp(-a) \sinh(|d|) \frac{d}{|d|} & 0 & 0 & \exp(-a) \cosh |d| \end{bmatrix}, \quad (\text{A } 12)$$

from which we obtain the expression for the partition function Z_G :

$$Z_G = 2 \exp(-a) \cosh |d| + 2 \exp a \cosh |b|. \quad (\text{A } 13)$$

For the expectation values given by equation (A 7) we obtain

$$\begin{aligned}
\xi_{zz} &= \frac{1}{Z_G} [2 \exp(-a) \cosh |d| - 2 \exp a \cosh |b|]; \\
\xi_{xx} &= -\frac{1}{Z_G} [2 \exp(-a) \sinh(|d|) \frac{1}{|d|} (\lambda_{xx} - \lambda_{yy}) + 2 \exp a \sinh(|b|) \frac{1}{|b|} (\lambda_{xx} + \lambda_{yy})], \\
\xi_{xy} &= -\frac{1}{Z_G} [2 \exp(-a) \sinh(|d|) \frac{1}{|d|} (\lambda_{xy} + \lambda_{yx}) + 2 \exp a \sinh(|b|) \frac{1}{|b|} (\lambda_{xy} - \lambda_{yx})], \\
\xi_{yx} &= -\frac{1}{Z_G} [2 \exp(-a) \sinh(|d|) \frac{1}{|d|} (\lambda_{xy} + \lambda_{yx}) + 2 \exp a \sinh(|b|) \frac{1}{|b|} (\lambda_{xy} - \lambda_{yx})], \\
\xi_{yy} &= -\frac{1}{Z_G} [-2 \exp(-a) \sinh(|d|) \frac{1}{|d|} (\lambda_{xx} - \lambda_{yy}) + 2 \exp a \sinh(|b|) \frac{1}{|b|} (\lambda_{xx} + \lambda_{yy})].
\end{aligned} \tag{A 14}$$

If we introduce the abbreviations

$$B = \xi_{xx} + \xi_{yy} - i(\xi_{xy} - \xi_{yx}), \quad D = \xi_{xx} - \xi_{yy} + i(\xi_{xy} + \xi_{yx}), \tag{A 15}$$

then with the help of equation (A 14) we obtain

$$B = -\frac{4}{Z_G} \exp a \sinh(|b|) \frac{b}{|b|}, \quad D = -\frac{4}{Z_G} \exp(-a) \sinh(|d|) \frac{d}{|d|}. \tag{A 16}$$

Taking into account that

$$|B| = \frac{4}{Z_G} \exp a \sinh(|b|), \quad |D| = \frac{4}{Z_G} \exp(-a) \sinh(|d|), \tag{A 17}$$

we find that

$$\frac{B}{|B|} = -\frac{b}{|b|}, \quad \frac{D}{|D|} = -\frac{d}{|d|}. \tag{A 18}$$

Now we introduce four new parameters M_i :

$$\begin{aligned}
M_1 &= 1 + \xi_{zz} + |D|, & M_2 &= 1 + \xi_{zz} - |D|, \\
M_3 &= 1 - \xi_{zz} + |B|, & M_4 &= 1 - \xi_{zz} - |B|,
\end{aligned} \tag{A 19}$$

in terms of which we can express the von Neumann entropy on the given observation level. Using equations (A 13), (A 14) and (A 17) we obtain

$$\begin{aligned}
M_1 &= \frac{4}{Z_G} \exp(-a + |d|), & M_2 &= \frac{4}{Z_G} \exp(-a - |d|), \\
M_3 &= \frac{4}{Z_G} \exp(a + |b|), & M_4 &= \frac{4}{Z_G} \exp(a - |b|).
\end{aligned} \tag{A 20}$$

The Lagrange multipliers λ_{kl} can be expressed as functions of the expectation values ξ_{kl} :

$$\exp a = \left(\frac{M_3 M_4}{M_1 M_2} \right)^{1/4}, \quad \exp(|b|) = \left(\frac{M_3}{M_4} \right)^{1/2}, \quad \exp(|d|) = \left(\frac{M_1}{M_2} \right)^{1/2}. \tag{A 21}$$

After inserting these expressions into equation (A 13) we obtain for the partition function

$$Z_G = \frac{4}{(M_1 M_2 M_3 M_4)^{1/4}}. \quad (\text{A } 22)$$

When we insert equations (A 18), (A 21) and (A 22) into equations (A 1), (A 4) and (A 12), then we find both the entropy

$$S_G = - \sum_{i=1}^4 \frac{M_i}{4} \ln \left(\frac{M_i}{4} \right) \quad (\text{A } 23)$$

and the GCDO

$$\hat{\rho}_G = \frac{1}{4} \begin{bmatrix} 1 + \xi_{zz} & 0 & 0 & D^* \\ 0 & 1 - \xi_{zz} & B^* & 0 \\ 0 & B & 1 - \xi_{zz} & 0 \\ D & & & 1 + \xi_{zz} \end{bmatrix} \quad (\text{A } 24)$$

as functions of the expectation values ξ_{kl} . Finally, we can rewrite the reconstructed density operator (A 24) in terms of the spin operators (see table 3).

A.2. Observation level $\mathcal{O}_H^{(2)}$

The GCDO on the $\mathcal{O}_H^{(2)}$ can be obtained as a result of a reduction of the observation level $\mathcal{O}_G^{(2)}$. The difference between these two observation levels is that the $\mathcal{O}_H^{(2)}$ does not contain the operator $\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)}$, that is the corresponding mean value is unknown from the measurement.

According to the maximum-entropy principle, the observation level $\mathcal{O}_H^{(2)}$ can be obtained from $\mathcal{O}_G^{(2)}$ by setting the Lagrange multiplier λ_{zz} equal to zero. With the help of the relation (see equation (A 7))

$$\lambda_{zz} = \frac{\partial S_G}{\partial \xi_{zz}} = - \frac{1}{4} \ln \left(\frac{M_1 M_2}{M_3 M_4} \right) = 0 \quad (\text{A } 25)$$

we obtain

$$M_1 M_2 = M_3 M_4. \quad (\text{A } 26)$$

From this equation we find the ‘predicted’ mean value of the operator $\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)}$ (i.e. the parameter t in table 3):

$$\xi_{zz} = \frac{1}{4}(|D|^2 - |B|^2) \equiv t. \quad (\text{A } 27)$$

Taking into account that the parameters $|B|$ and $|D|$ are given by

$$|B|^2 = (\xi_{xx} + \xi_{yy})^2 + (\xi_{xy} - \xi_{yx})^2, \quad |D|^2 = (\xi_{xx} - \xi_{yy})^2 + (\xi_{xy} + \xi_{yx})^2, \quad (\text{A } 28)$$

we can express the predicted mean value ξ_{zz} as a function of the measured mean values ξ_{xx} , ξ_{xy} , ξ_{yx} and ξ_{yy} :

$$\xi_{zz} = \xi_{xy}\xi_{yx} - \xi_{xx}\xi_{yy}. \quad (\text{A } 29)$$

When we insert equation (A 27) into equation (A 19) we obtain

$$M_1 = N_1 N_2, \quad M_2 = N_3 N_4, \quad M_3 = N_1 N_3, \quad M_4 = N_2 N_4, \quad (\text{A } 30)$$

where the parameters N_i are defined as

$$\begin{aligned} N_1 &= 1 + \frac{1}{2}(|D| + |B|), & N_2 &= 1 + \frac{1}{2}(|D| - |B|), \\ N_3 &= 1 - \frac{1}{2}(|D| - |B|), & N_4 &= 1 - \frac{1}{2}(|D| + |B|). \end{aligned} \quad (\text{A } 31)$$

In addition, from equations (A 30) and (A 23) we obtain the expression for the von Neumann entropy of the density operator reconstructed on the observation level $\mathcal{O}_H^{(2)}$:

$$S_H = - \sum_{i=1}^4 \frac{N_i}{2} \ln \left(\frac{N_i}{2} \right). \quad (\text{A } 32)$$

Finally, from equations (A 28) and (A 24) we find the expression for the GCDO on the observation level $\mathcal{O}_H^{(2)}$ (see table 3):

$$\begin{aligned} \hat{\rho}_H &= \frac{1}{4} [\hat{I}^{(1)} \otimes \hat{I}^{(2)} + (\xi_{xy}\xi_{yx} - \xi_{xx}\xi_{yy})\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)} \\ &+ \xi_{xx}\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)} + \xi_{xy}\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_y^{(2)} + \xi_{yx}\hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_x^{(2)} + \xi_{yy}\hat{\sigma}_y^{(1)} \otimes \hat{\sigma}_y^{(2)}]. \end{aligned} \quad (\text{A } 33)$$

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