

# On the problem of the theoretical identification of a physical entanglement in spins systems in the NMR quantum computation



J. D. Bulnes<sup>1</sup>, F. A. Bonk<sup>2</sup>

<sup>1</sup>Grupo de Mecânica Quântica, Informação Quântica e Física Aplicada, Universidade Federal do Amapá, Rod. Juscelino Kubitschek, Km. 2, Jardim Marco Zero, CEP. 68903-419, Macapá, AP, Brasil.

<sup>2</sup>Instituto de Ciências Exatas e Tecnologia, Universidade Paulista, Rua Miguel Guidotti, 405, Egisto Ragazzo, CEP.13485-342, Limeira, SP, Brasil

E-mail: bulnes@unifap.br

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## Abstract

The purpose of this paper is to present physical arguments that might justify the view that, in the problem of the theoretical identification of physical entanglement in the Nuclear Magnetic Resonance Quantum Computation (NMR-QC) of liquid solutions at room temperature, the bound of non-separability of Braunstein *et al.* (PRL, **83**, 1054 (1999)) it's not directly applicable to NMR nuclear spins systems (with  $I = 1/2$ ). Arguments such as the difference between mathematical entanglement and physical entanglement are considered.

**Keywords:** Quantum entanglement, Extended pseudo-pure matrix.

## Resumen

El objetivo de este artículo es presentar algunos argumentos físicos que puedan justificar el punto de vista de que en el problema de la identificación teórica del entrelazamiento cuántico en la Computación Cuántica por Resonancia Magnética Nuclear de soluciones líquidas a temperatura ambiente el límite de no separabilidad de Braunstein *et al.* (PRL, **83**, 1054 (1999)) no es aplicable directamente a los sistemas de espín nuclear RMN (con  $I = 1/2$ ). Se han considerado argumentos tales como la diferencia entre el entrelazamiento matemático y el entrelazamiento físico.

**Palabras clave:** Quantum, Matriz pseudo-pura extendida.

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## I. INTRODUCTION

The first mathematical results that would enable to identify the type of density matrix (separable or entangled) that corresponds to each one of the states of nuclear spin system in the experimental implementations of quantum protocols and quantum algorithm through the methods of liquid-state nuclear magnetic resonance quantum computing at room temperature performed until 1999 were obtained by Braunstein *et al.*, [1]. Specifically, it was shown that, to the case of  $N$  qubits and considering the parameter<sup>1</sup>  $\varepsilon$  of pseudo-pure matrices, the relation  $\varepsilon \leq 1/(1+2^{2N-1})$  constitutes a sufficient condition to the separability of  $N$  qubits's states and that the relation  $\varepsilon > 1/(1+2^{N/2})$  establishes a necessary condition to the non-separability of the corresponding state of  $N$  qubits. When the former conditions are used directly with

the values of the experimental parameters, for example, those of the experimental implementation made by Nielsen *et al.* about the quantum teleportation using NMR, [2], on which  $\varepsilon$  is approximately  $10^{-5}$  and  $N = 2$ , seem justifiable the following statements<sup>2</sup>: (1) "... *The bound show that no entanglement appears in the physical states at any stage of present NMR experiments...*" (Underlined by us), and (2)

"*Our results have implications for attempts to use high-temperature NMR techniques to perform quantum computations or other quantum-information-processing task. They imply that NMR experiments performed to date have not produced genuinely entangled density matrices.*" (Underlined by us).

Our purpose on this paper is to present and discuss arguments that may justify the opinion that the physical entanglement has not been characterized in [1], unless the *mathematical entanglement*, so that the non-separability

<sup>1</sup> That in the NMR experiments is defined by magnitudes as the temperature and strength of the magnetic field and with value in the interval  $\langle 0,1 \rangle$ .

bound in [1] it's not directly applicable to spins systems in NMR quantum computation experiments.

## II. 'MATHEMATICAL PROPERTIES' vs. 'PHYSICAL PROPERTIES' AND 'RESULTS CORRECTS BUT ONLY MATHEMATICAL vs. RESULTS WITH PHYSICAL MEANING'

The quantum mechanical model admits, truly, two types of entanglement: (i) The one that has physical meaning; that is, at first, it may be experimentally implemented on *qbits* of a compound quantum system, and (ii) the other that is only mathematical (or spurious); that is, that manifests uniquely as a quantum model property without being possible to establish any correspondence (with physical meaning) with some *qbits*'s systems property. The previous statement is supported in the examples of *mathematical entanglement* constructed<sup>3</sup> in [3, 4] and in the elucidation (of general character) made by Prugovecki, [5], who emphasized separation between formalism purely mathematical of the quantum model and the correspondences among the elements (and properties) of this formalism with the elements (and properties) of the modeled physical world.

Concretely, it can be states that: (a) each relevant physical property of the system or physical phenomenon under observation has a corresponding well-defined element (a mathematical property of a mathematical object) on a physical model; for example, the accessible energies for a quantum particle (on nature) submitted to a determine potential and the eigenvalues of determined Hermitian operator (on the model)<sup>4</sup>. On the other hand, (b) a mathematical property of a physical model will not have, necessarily, a corresponding property on nature; for example, the spin  $S = 0$  associated to the longitudinal sector of a four-dimensional field that obeys Maxwell's equations<sup>5</sup>.

In the first case, (a), it's said that the model property has *physical meaning* and, in the second case, (b), it's said that it is a property (mathematical) that is uniquely of the model.

On the other hand, a mathematically correct result, but without physical meaning, is that shown, for example, in

<sup>3</sup> In [4] a 4x4 entangled matrix with the form of a pseudo-pure matrix,  $\rho_\varepsilon = (1 - \varepsilon)I_4/4 + \varepsilon\rho_1$ , was built, in which the matrix  $\rho_1$  also is entangled. The entanglement was identified through the Peres-Horodecki criterion, but such entanglement it's not physical, but only mathematical.

<sup>4</sup> Another example: the symmetry of the physical potential and the degeneration of the eigenvalues of the energy operator; or, even, the breaking of the symmetry of the potential (perturbed by a small potential that doesn't have the symmetry of the initial potential) and the breaking of the degeneration (initial) of the eigenvalues of the energy operator.

<sup>5</sup> That component of spin is eliminated by a *principle of gauge*, but the component of spin  $S = 1$  is the one that corresponds to a physical property of the corresponding physical field.

[6], after supposing that the magnetic field gradient in a Stern-Gerlach apparatus is small and consider it as a perturbation of the homogeneous component (supposed intense) of the same field, one obtains, through the use of the perturbation theory, the expected spatial separation; nevertheless, according to the physical point of view, the right is an intense gradient<sup>6</sup> that produces the spatial separation of the incident beam (of the electrically neutral particles with spin  $S = 1/2$ ) in two beams .

## II. PHYSICAL ASPECTS NOT CONSIDERED ON LITERATURE ABOUT THE NMR PHYSICAL ENTANGLEMENT IDENTIFICATION PROBLEM

(I) Literature registers quantum entanglement as a property that manifests itself in a non-local and instantaneous manner among quantum particles (of a compound system) that are correlated, but uncoupled, without interaction, but interacted in the past. In the case of the particles that interact permanently, as an electron and a nuclei in an atom or particles with spin in a nuclei, a direct reference to physical entanglement<sup>7</sup> it would have to be considered precautionary.

In [8], for example, are described the measurements of correlations among ions  $^9\text{Be}^+$  that interacted intensely, it was justified that the active coupling didn't affect its entangled internal states. In [1] it was not incorporated any mathematical representation for the fact that the NMR spins interact permanently.

(II) In the so-called quantum protocols it's considered, implicitly, that the corresponding state spaces are unalterable throughout the implementation of any computational process. We remind you that when in a system of particles their parts don't interact the Hilbert's space to the full system it is defined by tensorial product of the associated spaces with the parts, but when these parts interact it's not correct to use the tensorial product, unless it is done just as a limited approximation in the case of very weak interactions.

Generally, by effect of an interaction, the spaces of underlying states may be modified. We can understand as a Hilbert's space may be modified considering a confined electron in a modeled device by a well of finite rectangular potential whose depth, in a determined instant, is " $-V$ ": The Hilbert's space changes from  $N$  - dimensional to  $(N + 1)$  - dimensional when the potential passes some value in the interval:

<sup>6</sup> The novelty with respect to the Stern-Gerlach effect, as it was shown in [7], it's that the Stern-Gerlach magnetic field gradient also contributes to the system energies.

<sup>7</sup> The statement that the entangled particles maintain in interaction independently of the distance that separates them, and, therefore, they must be considered as a unique system, they don't refer to a physical result, but to an *interpretation*.

$$\pi^2 \hbar^2 (N-1)^2 / 2ma^2 \leq V < \pi^2 \hbar^2 N^2 / 2ma^2$$

to other value in the interval:

$$\pi^2 \hbar^2 N^2 / 2ma^2 \leq V < \pi^2 \hbar^2 (N+1)^2 / 2ma^2$$

In such a described situation, the physical meaning attributed to the states may be lost, because nothing assures that an entangled state maintains that way to consider, if appropriate, Hilbert's space changing.

(III) In a theoretical analysis of the problem of the physical entanglement characterization among NMR spin it cannot be sufficient to consider, only, the form of pseudo-pure matrix,  $\rho_\varepsilon = (1-\varepsilon)I_n / 2^n + \varepsilon\rho_1$ , because, in this case, one cannot deny the fact of being considering only a *mathematical entanglement* of mathematical states. This way, it's essential to establish, if it's possible, the physical correspondences among the mathematical properties (of the theoretical results) and the physical properties (characteristics of the system considered), correspondences that cannot be reduced to the verification of the mathematical condition  $\varepsilon > 1/(1+2^{N/2})$ , because it was obtained without considering the physics of the problem, ignoring the implements characteristics in the experiments of Nuclear Magnetic Resonance Quantum Computing.

## VI. CONCLUSIONS

Considering that in the development presented in [1] it wasn't incorporated any significant physical characteristics of the NMR spins systems nor of the NMR quantum computing experiments, as, for example, the situation in which only a part of the  $N$  spins could be entangled, we have focused in physical aspects omitted on this development. Specifically, we have identify as absent in the mathematical treatment of the problem of theoretical identification of a physical entanglement among NMR spins, the following subjects: an approach that distinguishes between the situation when the particles interact and when they don't interact; the possibility that the space of physical states may result modified; a distinction between the mathematical entanglement and the physical entanglement,

*On the problem of the theoretical identification of a physical entanglement...*

and, finally, the establishment of correspondences with physical meaning.

We conclude that:

(i) The mathematical context defined in [1], when it's not considered any complement, only permits apply it to a mathematical entanglement of mathematical states, and that, (ii) the non-separability bound in [1] couldn't discard (at first, and if it was the case) a physical entanglement among NMR spins in the NMR quantum computing experiments. We emphasize on necessity that verifies complementariness, which only could be of an experimental nature, must be implemented to decide if a state has associated, in correspondence, a physical entanglement.

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