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► **To cite this version:**

Gilbert Reinisch. Mixed-state density operator in a nonlinear quantum system: Erratum. *Annals of Physics*, 2025, 476, pp.169979. <10.1016/j.aop.2025.169979>. <hal-04979366>

HAL Id: hal-04979366

<https://hal.science/hal-04979366v1>

Submitted on 6 Mar 2025

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Mixed-State Density Operator in a Nonlinear Quantum System: erratum

Gilbert Reinisch*

*Université de la Côte d'Azur - Observatoire de la Côte d'Azur
06304 Nice Cedex - France*

Abstract

In *G. Reinisch, Annals of Phys., 449, (2023) 169205*, a significant error was made regarding the definition of the base of density matrix ρ . This led to an erroneous expression of the only adjustable degree of freedom in our nonlinear quantum model. This article corrects this error and accordingly rewrites the analytical part of the previous incorrect paper.

PACS numbers: 73.21.La 71.10.Li 71.90+q

*Electronic address: Gilbert.Reinisch@oca.eu

Nonlinear quantum eigenstates are usually non-orthogonal and can therefore lead to stunning physical properties. Being as a rule non-Hermitian in flat spaces, they may become Hermitian in curved spaces [1]. Another intriguing example is the nonlinear Schrödinger-Poisson (SP) quantum system whose eigenstate transitions due to non-orthogonality can fit quantum electrodynamics [2]. This physical property yields an ab-initio nonlinear quantum definition of the fine-structure constant's value $\sim 1/137$ [3] [4] which is “*one of the greatest damn mysteries of physics*” according to Feynman [5]. Strong nonlinearities allow such SP systems to become Thomas-Fermi classical [6]. The case where the density of states varies rapidly with energy can be described by a stable algorithm [7].

Consider two nonlinear quantum eigenstates $|i\rangle$ and $|j\rangle$ and their respective eigenvalues — or chemical potentials— μ_i and $\mu_j \neq \mu_i$ [8]. We use parenthesis for the nonlinear eigenstates, e.g. $|i, j\rangle$, and kets for linear orthonormal eigenstates : e.g. $|i, j\rangle$. The non-zero overlap amplitude (or non-orthogonality) $(i|j) = \int u_i^* u_j d\mathbf{x} \neq 0$ defined by the respective wave functions $u_{i,j}(\mathbf{x})$ can be related to the well-known concept of quantum mixed-state [9]. This latter is obtained by statistically combining the nonlinear eigenstates $|i, j\rangle$ with appropriate normalized probabilities $p_{i,j} > 0$ such that $p_i + p_j = 1$. The problem consists in finding the probabilities $p_{i,j}$. In [8], we were looking for the corresponding density operator ρ . However the definition of ρ demands a statistical mixture of orthonormal states. Therefore we defined Löwdin's symmetrically-orthonormalized base $|i, j\rangle$ from the original nonlinear eigenstates $|i, j\rangle$ [10] and diagonalized it, yielding $p_{i,j}$ as its positive eigenvalues. However, we made the error of defining this diagonal density matrix in Löwdin's orthogonal basis $|i, j\rangle$ instead of using it in the original nonlinear basis $|i, j\rangle$. The aim of the present paper is to correct this error.

The generalization is straightforward for $n > 2$ discrete nonlinear and non-orthogonal eigenstates. Then the $n \times n$ overlap matrix yield Löwdin's n symmetrically-orthonormalized states which in turn define the $n \times n$ density matrix ρ whose diagonalization yield the n normalized probabilities of the mixed state. For the sake of clarity, we have illustrated procedure by use of the simplest case of a two-level nonlinear system because it is both easily analytically tractable and it nevertheless displays the main properties of the model. Moreover, it is experimentally sound: e.g. the “*s*” states of two-electron quantum-dot helium [11] [12].

To be specific [8], assume that the wave functions $u_{i,j}(\mathbf{x})$ of the nonlinear normalized eigenstates $|i\rangle$ and $|j\rangle$ corresponding to the respective nonlinear eigenvalues μ_i and μ_j are real-valued. Define the eigenstate non-orthogonality $A = (i|j) = (j|i) = \int u_i u_j d\mathbf{x} = S_{ij} = S_{ji}$ where the overlap matrix \mathbf{S} is defined by:

$$\mathbf{S} = \begin{pmatrix} 1 & A \\ A & 1 \end{pmatrix} \quad ; \quad \mathbf{S}^{-1/2} = \frac{\pm 1}{\sqrt{1-A^2}} \begin{pmatrix} \cos \theta & -\sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \quad ; \quad \mathbf{S}^{1/2} = \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \quad , \quad (1)$$

and $A = \sin 2\theta$. Löwdin's symmetrically-orthonormalized states are [10]:

$$\begin{pmatrix} |i\rangle \\ |j\rangle \end{pmatrix} = \mathbf{S}^{-1/2} \begin{pmatrix} |i\rangle \\ |j\rangle \end{pmatrix} \quad . \quad (2)$$

Note that, due to nonlinearity, these states are not *eigenstates* —nor even solutions— of the nonlinear differential quantum system (say, Schrödinger-Poisson or Gross Pitaevskii for instance). They will serve as intermediate tools to unambiguously define the density matrix in the nonlinear eigenstate basis $|i, j\rangle$. Indeed, we look for a 2×2 matrix ρ

in Löwdin's orthonormalized base states Eq. 2 whose diagonalization by use of this errary transformation would yield:

$$\boldsymbol{\rho}_{\text{diag}} = \mathbf{S}^{1/2} \boldsymbol{\rho} \mathbf{S}^{-1/2} = \begin{pmatrix} p_i & 0 \\ 0 & p_j \end{pmatrix} . \quad (3)$$

Matrix $\boldsymbol{\rho}_{\text{diag}}$ provides a sound definition of a density matrix in the nonlinear quantum system defined by eigenstates $|i, j\rangle$ as shown later by Eq. 6. Eigenvalues $p_{i,j}$ are the respective normalized statistical weights —or respective populations— for both nonlinear eigenstates $u_{i,j}$.

The solution that includes a free parameter α is found to be:

$$\boldsymbol{\rho} = \begin{pmatrix} \alpha & A(\alpha - \frac{1}{2}) \\ -A(\alpha - \frac{1}{2}) & 1 - \alpha \end{pmatrix} . \quad (4)$$

with

$$p_i = \frac{1}{2} \pm (\alpha - \frac{1}{2})\sqrt{1 - A^2} \quad ; \quad p_j = \frac{1}{2} \mp (\alpha - \frac{1}{2})\sqrt{1 - A^2} . \quad (5)$$

The \pm sign in Eq. 5 is redundant: it defines two actually equivalent solutions that only depend on eigenstate labelling. Therefore we adopt in the following the positive sign. Parameter α together with non-orthogonality parameter $A = (i|j)$ are the only adjustable degrees of freedom in order to fit with experimental data.

Consider for example Hamiltonian \mathbf{H} in the nonlinear basis $|i, j\rangle$ where $\mu_{i,j}$ are its eigenvalues:

$$\mathbf{H} = \begin{pmatrix} \mu_i & 0 \\ 0 & \mu_j \end{pmatrix} . \quad (6)$$

Its quantum expectation value reads, in accordance with Eqs 3, 5 and 6 related to the nonlinear basis $|i, j\rangle$:

$$E = \text{Tr}[\boldsymbol{\rho}\mathbf{H}] = p_i\mu_i + p_j\mu_j = \frac{1}{2}(\mu_i + \mu_j) + (\alpha - \frac{1}{2})\sqrt{1 - A^2}(\mu_i - \mu_j) . \quad (7)$$

By writing \mathbf{H} in Löwdin's orthonormalized basis (2):

$$\mathbf{S}^{-1/2} \mathbf{H} \mathbf{S}^{1/2} = \frac{1}{\sqrt{1 - A^2}} \begin{pmatrix} \mu_i \cos^2\theta - \mu_j \sin^2\theta & \frac{A}{2}(\mu_i - \mu_j) \\ -\frac{A}{2}(\mu_i - \mu_j) & \mu_j \cos^2\theta - \mu_i \sin^2\theta \end{pmatrix} . \quad (8)$$

and taking the trace of this Hamiltonian times the corresponding density matrix $\boldsymbol{\rho}$ given by Eq. 4, we verify that we obtain again energy (7). This latter yields the definition of the unknown parameter α :

$$\alpha = \frac{1}{2} + \frac{\frac{1}{2}(\mu_i + \mu_j) - E}{\sqrt{1 - A^2}(\mu_j - \mu_i)} . \quad (9)$$

As an example, consider the quantization of C^{4+} carbon ion in the two-electron Coulomb system [13] (where $Z = 6$ and *a.u.* means atomic unit in this reference). Eigenstate overlap $A = (i|j) = -0.05$ and the nonlinear eigenvalue (or chemical potential) of the ground state is $\mu_i = -0.40059 \text{ a.u.}/Z^2$ while we have $\mu_j = -0.1007 \text{ a.u.}/Z^2$ for the first excited state. The corresponding experimental value is $E = -0.40023 \text{ a.u.}/Z^2$. Therefore Eqs 9 and 5

respectively yield $\alpha = 0.9994$ and $p_i = 0.9988$, $p_j = 0.0012$ while the density matrix ρ in the orthonormalized basis (4) is quite close to

$$\rho = \begin{pmatrix} 1 & A/2 \\ -A/2 & 0 \end{pmatrix} . \quad (10)$$

Actually, for most nonlinear quantum systems (e.g. Coulombian [13] or parabolic [14] electron-pair confinement), we have: $A^2 \sim 10^{-2}$ or less. Then:

$$p_i \sim \alpha + o(A^2) \quad ; \quad p_j \sim 1 - \alpha + o(A^2) . \quad (11)$$

We recover Eq. 6 of article [8] and therefore its consequences developed in the rest of this article although the density matrix ρ given by Eq. 4 was wrongly considered as defined in the nonlinear basis $|i, j\rangle$.

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