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The emergence of classical mixtures from an entangled quantum state **FREE**

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The emergence of classical mixtures from an entangled quantum state

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This note advocates for a pedagogical approach that illustrates by a simple example how what appear to be classical mixtures arise in a quantum subsystem of a purely quantum state. I show below how measuring one particle of two entangled spin-1/2 particles yields an expectation value that takes the form of a population average, hinting at the general principle that what appear to be classical probabilities emerge from pure quantum states. In contrast, the standard textbook approach uses the possibility that a quantum system is in an apparent mixture of classical states to motivate the density matrix without explaining how classical mixtures may arise. Through a simple example like the one discussed here, one may explain that entanglement with the environment results in such mixtures.

The fact that mixtures are a general consequence of a quantum subsystem is stressed by Landau and Lifshitz¹ “...it would be quite incorrect to suppose that the description by means of the density operator signifies that the subsystem can be in various Ψ states with various probabilities and that averaging is over these probabilities. Such a treatment would be in conflict with the basic principles of quantum mechanics.” This interaction of a quantum system with its environment is the basis of quantum noise² and decoherence,^{3,4} which are important modern topics for students to understand.

This emphasis is lacking in the most-often used quantum mechanics textbooks.^{5–12} The simple two-spin-1/2 system I use here can be found in the *Afterward* of the textbook by Griffiths and Schroeter,¹³ but the authors otherwise use the standard approach. Only at the very end do they come back to the state vector but do not show how the density matrix emerges from it as a purely quantum phenomena. The approach introduced in this Note avoids the density matrix altogether, illustrating how the mixed state results directly from the state vector. Cohen-Tannoudji, Diu, and Laloë present an abstract derivation of a quantum subsystem with no simple example and do so only *after* developing the density operator.⁹ My suggested approach establishes the intuitive foundations from the quantum perspective to motivate the density matrix.

Textbooks start by introducing single-particle eigenstates. Then, superposition states such as

$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle \quad (1)$$

are introduced, where $|\alpha|^2 + |\beta|^2 = 1$ and $|\uparrow\rangle$ and $|\downarrow\rangle$ are spin states with spins $\pm 1/2$, respectively. For the state given in Eq. (1), the probability of detecting a spin up electron is given by the Born rule,

$$\mathcal{P}_\uparrow = |\langle\uparrow|\psi\rangle|^2 = |\alpha|^2. \quad (2)$$

Next, the expectation value is defined. For the state given in Eq. (1), the expectation value of operator A is

$$\begin{aligned} \langle\psi|A|\psi\rangle &= |\alpha|^2\langle\uparrow|A|\uparrow\rangle + |\beta|^2\langle\downarrow|A|\downarrow\rangle \\ &\quad + \alpha^*\beta\langle\uparrow|A|\downarrow\rangle + \beta^*\alpha\langle\downarrow|A|\uparrow\rangle. \end{aligned} \quad (3)$$

The first two terms of Eq. (3) include the coefficients $|\alpha|^2$ —the probability of finding spin up electrons; and $|\beta|^2$ —the probability of spin down electrons, consistent with the classical notion of weighted averages. The last two terms come from quantum interference, which can cause destructive (or constructive) interference leading to an expectation value that is smaller (or larger) than the sum over the contributions from each state alone. Alternatively, the cross terms that are responsible for interference can be the only ones that contribute when the “classical” terms vanish. The operator $A = S_x$ is such an example, where $S_x = (\hbar/2)(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|)$. Equation (3) then has only nonzero off-diagonal elements and yields

$$\langle\psi|S_x|\psi\rangle = \frac{\hbar}{2}(\alpha\beta^* + \alpha^*\beta). \quad (4)$$

Thus, quantum interference originates in the off-diagonal elements of an observable and can be nonzero even when both states individually do not contribute.

Textbooks then solve the single-particle Schrödinger equation for one-dimensional potentials and central potentials, develop angular momentum and spin, and solve the hydrogen atom. Subsequently, the density operator is introduced. I propose that the two-particle state vector be introduced first to show how the density operator and mixtures naturally emerge for a one-particle subsystem.

The reader should keep in mind that, throughout this letter, we are interested in the spin of *one electron*, be it the single electron described in Eq. (1) or one electron that is entangled with another one (or many others) acting as its environment, as I describe below.

We introduce the two-electron spin state $|\uparrow\rangle|\downarrow\rangle$ to mean that the leftmost ket corresponds to electron #1, which has spin 1/2 and electron #2’s ket is to the right with spin $-1/2$.

The state vector $|\uparrow\rangle|\downarrow\rangle$ cannot represent two indistinguishable particles because it uniquely labels each particle by its eigenvalue: Electron #1 has spin 1/2 and electron #2 has spin $-1/2$. However, the linear combination¹⁴

$$|\uparrow, \downarrow\rangle = \frac{1}{\sqrt{2}} [|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2] \quad (5)$$

makes the electrons indistinguishable (each electron is in both spin states so cannot be uniquely identified by an eigenvalue),¹⁵ and expectation values are unchanged when the electrons are interchanged. Though redundant, subscripts that label particle number are added for emphasis.

Interestingly, each term in Eq. (5) distinguishes between the two electrons, yet when added together, the state $|\uparrow, \downarrow\rangle$ does not. At this point, the student learns that Eq. (5) defines an entangled state, which cannot be expressed as a product of two single-electron state vectors $|\psi\rangle_1|\phi\rangle_2$.

For the state given in Eq. (5), the probability that electron #1 is in the up spin state $\mathcal{P}_\uparrow^{(1)}$ is again given by the Born rule,

$$\mathcal{P}_\uparrow^{(1)} = |(\langle\uparrow|_1 \mathbb{1}_2)|\psi\rangle|^2 = \left| \frac{1}{\sqrt{2}}|\downarrow\rangle_2 \right|^2 = \frac{1}{2}, \quad (6)$$

where the bra $\langle\uparrow|_1$ acts only on the first electron and the identity $\mathbb{1}_2$ leaves the state of electron #2 unchanged. So, when operating on $|\uparrow\rangle|\downarrow\rangle \equiv |\uparrow\rangle_1|\downarrow\rangle_2$ yields the ket $|\downarrow\rangle_2$. This is the same probability as given in Eq. (2) when $\alpha = \beta = 1/\sqrt{2}$ —the case where the superposition contains equal parts of up and down spin states.

Next we calculate the expectation value of a single particle operator that lives in the space of electron #1. This operator takes the form $A_1 \equiv A_1 \mathbb{1}_2$, where the identity $\mathbb{1}_2$ acts on electron #2. With the two-electron state vector $|\Psi\rangle = |\uparrow, \downarrow\rangle$, the operator A_1 acts on the first electron (leftmost ket in each term) while leaving the state of the second one unchanged, leading to the expectation value

$$\begin{aligned} \langle\Psi|A_1|\Psi\rangle &= \frac{1}{2}(\langle\uparrow|A_1|\uparrow\rangle\langle\downarrow|\downarrow\rangle + \langle\downarrow|A_1|\downarrow\rangle\langle\uparrow|\uparrow\rangle \\ &\quad - \langle\uparrow|A_1|\downarrow\rangle\langle\downarrow|\uparrow\rangle - \langle\downarrow|A_1|\uparrow\rangle\langle\uparrow|\downarrow\rangle) \\ &= \frac{1}{2}\langle\uparrow|A_1|\uparrow\rangle + \frac{1}{2}\langle\downarrow|A_1|\downarrow\rangle. \end{aligned} \quad (7)$$

Note that indistinguishability requires $\langle\Psi|A_1|\Psi\rangle = \langle\Psi|A_2|\Psi\rangle$. Equation (7) with $A_1 = S_{x1}$ gives

$$\langle\Psi|S_{x1}|\Psi\rangle = 0, \quad (8)$$

which is different than the single-particle result of Eq. (4).

The parallel derivations leading from Eq. (1) to Eq. (4) and the one leading from Eq. (5) to Eq. (8) tells the whole story, as follows. Assume that $\alpha = \beta = 1/\sqrt{2}$ from here on. Equation (1) describes a single electron in a superposition of two states with equal parts of spin up and spin down. Equation (5) describes two entangled electrons, each having equal parts of spin up and spin down. For both systems, we seek the properties of one of the electrons. In the two-electron case, the one being measured can be viewed as the subsystem of the two-electron state with the other one as the environment.

According to Eqs. (2) and (6), a measurement of the spin of one electron in both cases yields spin up half the time. In contrast, the expectation value of the spin given in Eqs. (4) and (8) is different even though in both cases, spin up and spin down are found in equal proportions. This may appear puzzling given that the particles are assumed to not interact. So how does the presence of the second electron affect the properties of the first one? The answer is through entanglement. All identical spin-1/2 particles, such as electrons, must be entangled,¹⁶ and for two particles when there are no other

degrees of freedom, the spin part of state vector must take the form of Eq. (5). The presence of the second particle removes the interference contribution to the expectation value, giving what one expects for a classical mixture. The student should focus on these two parallel developments to gain insights into how entanglement and superposition differ with regard to the behavior of a single particle and how these manifest in what is measured for that single particle.

Such simple calculations can be used as a learning aid to appreciate the consequences of entanglement, to understand the difference between superposition and entanglement and to stress the futility of separating a system from its environment in the classical way with distinct and obvious boundaries.

Equation (7), though fully quantum in nature, hints at a classical interpretation with half of the electrons in the spin-up state contributing

$$\frac{1}{2}\langle\uparrow|A_1|\uparrow\rangle$$

to the expectation value and the other half of the electrons in the spin down state contributing

$$\frac{1}{2}\langle\downarrow|A_1|\downarrow\rangle.$$

Indeed, the introduction of the density operator typically starts with the expectation value of the operator A ,

$$\langle A \rangle = \sum_i w_i \langle i|A|i \rangle, \quad (9)$$

where w_i is interpreted as the fraction of particles in single-particle state $|i\rangle$ and $\langle i|A|i\rangle$ is the quantum expectation value of observable A for a particle in state $|i\rangle$.

Prior to the formal introduction of mixtures, we are taught that the state vector contains all the physics. Subsequently, many textbooks motivate density matrices as a means for treating classical mixtures using Eq. (9) as the starting point, which throughout the narrative implies the need for auxiliary information outside of quantum probabilities contained in the “classical population fractions” w_i . This implies a hybrid classical/quantum theory. Imagine Eq. (9) being the first introduction to mixtures.

The quantum origins of w_i through entanglement with the environment would be unapparent, and the student would be primed for the population fraction interpretation. A small number of textbooks, such as Griffiths and Schroeter,¹³ mention the two-particle example after introducing mixtures with the density matrix, but do not follow through with the calculations presented here, which is critical to getting the point. Use of the one-particle subsystem of a two-particle quantum state prior to introducing mixtures, as done here, clearly shows that the $1/2$ coefficients originate from the $1/\sqrt{2}$ factor in Eq. (5), which carries through to Eq. (7) when evaluating the expectation value of one of the particles in the two-particle system. Orthogonality between the states in the environment as seen in the second line of Eq. (7) removes the quantum interference terms to make a mixed state.

This simple two-particle example instills the kind of understanding held by experienced physicists, empowers the

novice to grasp the centrality of quantum mechanics, and engenders an appreciation of how the density operator emerges from a fully quantum system when we measure the properties of a part of that system.

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AUTHOR DECLARATIONS

Conflict of Interest

To the best of his knowledge, the author has no conflict of interest to disclose.

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¹⁴Note that $|\psi, \phi\rangle$, defined in Eq. (5) with $|\psi\rangle$ and $|\phi\rangle$ each in superposition of the form given in Eq. (1) gives $|\psi, \phi\rangle = |\uparrow, \downarrow\rangle$ for all $|\psi\rangle$ and $|\phi\rangle$ when $|\psi\rangle \neq |\phi\rangle$.

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