Entangled Systems: Bell Inequality Violations, Entropy, and Environmental Monitoring via Density Matrix Calculations

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Abstract

This paper deals with a fundamental influence governing physical interaction: quantum entanglement. Its purpose is to present a physical, mathematical, and philosophical introduction to entanglement. To this end, entanglement is introduced via the EPR paradox, local hidden variable models, and Bell/CHSH inequalities. The EPR-Bohm pair is used throughout this paper as an example of an entangled system.

Density matrices are introduced as a fundamental mathematical tool for examining entangled systems. They are utilized to determine the theoretical maximal violation of the Bell and CHSH inequalities ($1.5 \leq 1$ and $2\sqrt{2} \leq 2$, respectively) for an optimal experimental setup emitting EPR pairs. For a setup emitting Werner states (i.e. EPR pairs coupled with classical noise) the minimum fidelity for violation of the Bell and CHSH inequalities is found to be $f = \frac{2}{3}$ and $\frac{\sqrt{2}}{2}$, respectively. Density matrices are also shown to be useful in calculating measures of entanglement, such as the von Neumann entropy.

Finally, the paper culminates in a consideration of systems entangled with the environment. This allows us to consider the role of entanglement in the quantum-to-classical transition.

This paper represents my own work in accordance with University regulations.

1 Introduction

The "paradox" is only a conflict between reality and
your feeling of what reality "ought to be."
Richard P. Feynman

...quantum phenomena do not occur in a Hilbert space,
they occur in a laboratory...
Asher Peres

The development of quantum theory in the early 1900s posed fundamental questions about physical interaction, questions of stunning philosophical implication that took physicists decades to begin to unravel. Central among these was a vexing lack of determinism at subatomic scales, a feature some took not to be a fundamental feature of nature, but rather proof of the incompleteness of quantum mechanics. Physical experiment showed certain quantum variables to be statistically understandable, but apparently unknowable for any given trial. As such, quantum mechanics was developed to be a statistical description of physical systems.

Not only were certain variables complementary, but isolated quantum systems showed distinctly nonclassical behavior. Particles behaved as waves, EPR pairs seemed to be nonlocally correlated over vast distances, and no one could satisfactorily explain if Schrödinger's cat was dead or alive. This behavior was complicated by the notion of a classical measurement: many physicists held notions of "wave collapse," or the supernatural effects of the "Heisenburg cut" between classical apparatus and quantum system. Yet these phenomena can all be explained by the distribution of coherence in quantum systems.

This paper presents a physical, mathematical, and philosophical introduction to entanglement. Section 2 introduces the concept of entanglement via the EPR paradox, local hidden variable theories, and Bell inequalities. Using the example of an EPR pair in the Bell state, we calculate the optimal experimental setup to violate the Bell and CHSH inequalities. The physical implications of these violations are then discussed.

Section 3 introduces pure and mixed state density matrices as a tool for examining entanglement. The EPR pair is shown to be in a pure state. The Werner state is then introduced as a mixed state extension of the Bell state. This serves as a realistic model for the noise in hypothetical Bell test experiments for an electron-positron pair. We then use the density matrix formalism in Section 4 to determine the necessary fidelity of the Bell state component of the Werner state for the same Bell and CHSH inequality tests.

Section 5 examines the entropy of entanglement. Purity and von Neumann entropy are given as measures of entanglement. This connects to the decoherence of quantum systems in contact with the environment, as discussed in Section 6.

2 Entangled Systems

2.1 Coherence and Decoherence

On the quantum scale, all matter exhibits a wave-particle duality. Coherence is the phenomenon of wave-like interference between systems, or even within a system. Coherence is the superposition of quantum states.

Entanglement is a subset of coherence in which systems became entangled via local interaction. Yet, remarkably, this interaction may still tie the systems together even if they become time- and space-like separated. In this sense, entanglement is shared coherence between systems. This coherence does not disappear as systems become more entangled with their environments; rather, decoherence is being "spread thin" by entanglement over a higher number of degrees of freedom. This relates entanglement to thermodynamic entropy, an influence that propagates the disorder of systems. Once systems become entangled, it is difficult to reverse their shared coherence. Entanglement is therefore responsible for the gradual quantum-to-classical transition that results in classical world of our everyday experience.

2.2 EPR Pair

Entanglement is best illustrated by the famous EPR paradox. In 1935, Albert Einstein partnered with two colleagues at the Institute for Advanced Study, B. Podolsky and N. Rosen, to publish a *gedanken* experiment challenging the completeness of quantum mechanics [1]. While EPR were primarily concerned with the philosophical arguments inherent in the paradox, we shall first examine the system itself so as to introduce entanglement.

A simple example of an "EPR Pair" is given by Bohm [2]: A neutral pi meson of spin zero decays into a positron and electron, such that the resultant particles fly off in opposite directions. We consider both the electron and positron.

We often describe a single particle with a single wave function, giving the statistical distribution of behavior for that single particle. Such a function expressing complete information about the system is a *pure state*. In this case we are interested in spin, and choose a two-dimensional orthogonal basis for spin up and down as

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \uparrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \downarrow \tag{1}$$

Since quantum mechanics always allows us to write the state of a system as a linear superposition of basis states,

$$|\psi\rangle = \sum_i c_i |\psi_i\rangle \tag{2}$$

a single particle equally likely to be spin up or down can be written simply as

$$|\psi\rangle = \frac{1}{\sqrt{2}}(\uparrow + e^{i\phi} \downarrow) \tag{3}$$

for an arbitrary phase ϕ. A composite system requires a basis of higher dimensionality. For instance, a wave function describing the spins of both particles in the EPR pair must be four-dimensional. This basis is described by

$$|\psi\rangle = |\alpha\rangle_1 |\beta\rangle_2 = |\alpha_1 \beta_2\rangle \tag{4}$$

Here the subscript refers to the particle; the first particle is in state $|\alpha\rangle$, the second in state $|\beta\rangle$. Thus any number of particles can be described as an outer product of the individual basis states of each particle.

Returning to the EPR pair, conservation of angular momentum holds that the spins of the electron (-) and positron (+) must be opposite. However, we cannot tell which particle is spin up or spin down before measurement. If we measure the electron as spin down, we know that the positron is spin up without measurement. This makes clear the meaning of entanglement: no matter how far apart the electron and positron fly away from each other, their spins are entangled (until either particle comes into contact with other matter). This distance can be arbitrarily large (as large as the universe!) and entanglement will still hold. In this case, it is impossible to describe the particles individually. They can only be described together by a single wave function, a wave function that must still give the statistical distribution that each particle is in either spin state 50% of the time, and that angular momentum is conserved to zero. Quantum mechanics thus gives us the singlet wave function to describe particles *together* as being in a superposition of states,

$$|\psi_{+,-}\rangle = \frac{1}{\sqrt{2}}(\uparrow_+\downarrow_- - \downarrow_+\uparrow_-) \tag{5}$$

Mathematically, this superposition is rooted in the linearity of the Hilbert space its basis occupies. Physically, it reflects the fact that neither particle is fully in either spin state: each particle is in an antisymmetric superposition of both spin states. Eq. (5) is commonly called a Bell state because the two particles are maximally entangled, as shall be discussed in Section 5.1.

2.3 EPR Paradox

Such a conclusion is not immediately obvious. Ironically, EPR used this example to come to the opposite conclusion, the "realist" belief that the spins of the particles are fully defined from the instant of meson decay. EPR gave the following two-part definition of the completeness of a physical theory, a standard that quantum mechanics does not satisfy:

1. Condition of Completeness: "Every element of the physical reality must have a counterpart in the physical theory" [1].

2. Condition of Locality: Nature is fundamentally local, and thus any physical theory must also be local.

EPR's first condition rests on the following definition of an element of reality: "If, without in any way disturbing a system, we can predict with certainty (i.e., with probability equal to unity) the value of a physical quantity, then there exists an element of reality corresponding to this physical quantity" [1]. Put most simply, classic physics is a complete theory because, with absolute certainty, we can know the position, velocity, angular momentum, etc. of a given object. Quantum mechanics, however, cannot satisfy this requirement.

Returning to Bohm's EPR pair, there are two possibilities as to the physical reality of our system. The first is the realist position: that the spins of the two particles are fully defined from the instant of meson decay. When we measure the spin of the electron, it has absolutely no effect on the spin of the positron. In this case, it must be possible to satisfy the Condition of Completeness by adding "hidden variables" to the quantum theory. Just because we could not experimentally determine spins before measurement, didn't mean that there could not be a deterministic theoretical framework.

The second scenario links the spins of the two particles via entanglement. In "orthodox" language, the measurement of one particles spin also collapses the wave function of the other particle's spin. In this scenario, EPR thought it possible to measure the electron spin, and then measure the positron spin *before the influence of the electron spin measurement determined the positron spin.* Such a scenario would, in half of the experimental trials, produce identical spin measurements for both particles, thus violating conservation of angular momentum. This conclusion rests on the Condition of Locality: it would only be possible for the electron and positron spins to be entangled *if the influence of entanglement propagated faster than the speed of light.* To Einstein, the father of relativity, such superluminal velocity seemed an impossibility.

2.4 Bell's Inequality

EPR's famous paper closes with their belief that "a [complete] theory is possible," a suggestion that drove a generation of physicists to find a modification of quantum mechanics, or even an entirely new theory, by which the realist position could be championed. No one doubted that quantum mechanics was correct, only that it could be improved upon. This led to generations of physicists searching for so-called "hidden variable" theories: a quantum theory that could show, or at least explain, the experimentally viewed statistical nature of quantum physics. The hidden variable(s) λ were some unknown set of extra parameters that, in addition to the wave function, would fully characterize a quantum system.

Such efforts were heavily pursued until 1964 when the young John Bell published his proof of the incompatibility of quantum mechanics with *any* local hidden variable model (LHVM). Bell modified the EPR experiment such that the measurement apparatus of the electron and positron spins could be oriented at random, along axes independent of one another. Regardless of the orientation of the detector, it will measure the spin of a particle as ± 1, in units of $\hbar/2$. The introduction of λ allows for complete knowledge of whether the value is positive or negative in any given instance for any orientation of the measurement apparatus. Separating $\Psi_{e,p}$ this gives

$$\Psi_e(\mathbf{a},\lambda) = \pm 1, \Psi_p(\mathbf{b},\lambda) = \pm 1 \tag{6}$$

for arbitrary unit alignment vectors **a** and **b** for an apparatus. It is not obvious how arbitrarily aligning the two measurement apparatuses shows entanglement, as for a given trial the two spin measurements may only yield the values ± 1. Bell, however, proposed taking the average of the product of the results of the two measurements, $P(\mathbf{a},\mathbf{b})$. In the original EPR configuration, the two measurement apparatuses are aligned, thus

$$P(\mathbf{a},\mathbf{a}) = -1 \tag{7}$$

a prediction in agreement with quantum mechanics. If the detectors are antialigned, $P(\mathbf{a},-\mathbf{a}) = +1$. In other words,

$$\Psi_e(\mathbf{a},\lambda) = -\Psi_p(\mathbf{a},\lambda) \tag{8}$$

In general, quantum mechanics gives for the singlet

$$P(\mathbf{a},\mathbf{b}) = -\mathbf{a}\cdot\mathbf{b} = -\cos(\theta_{ab}) \tag{9}$$

Yet in a hidden variable theory, we have the probability distribution $\rho(\lambda)$ to determine "the expectation value of the product of the two" [3] spins

$$P(\mathbf{a},\mathbf{b}) = \int \rho(\lambda)\Psi_e(\mathbf{a},\lambda)\Psi_p(\mathbf{b},\lambda)\mathrm{d}\lambda \tag{10}$$

Using Eq. (8), this simplifies to

$$P(\mathbf{a},\mathbf{b}) = -\int \rho(\lambda)\Psi_e(\mathbf{a},\lambda)\Psi_e(\mathbf{b},\lambda)\mathrm{d}\lambda \tag{11}$$

Introducing another unit vector **c**,

$$\begin{aligned} P(\mathbf{a},\mathbf{b}) - P(\mathbf{a},\mathbf{c}) &= -\int \rho(\lambda)[\Psi_e(\mathbf{a},\lambda)\Psi_e(\mathbf{b},\lambda) - \Psi_e(\mathbf{a},\lambda)\Psi_e(\mathbf{c},\lambda)]\mathrm{d}\lambda \qquad (12) \\ &= -\int \rho(\lambda)[1 - \Psi_e(\mathbf{b},\lambda)\Psi_e(\mathbf{c},\lambda)]\Psi_e(\mathbf{a},\lambda)\Psi_e(\mathbf{b},\lambda)\mathrm{d}\lambda \qquad (13) \end{aligned}$$

since $[\Psi_e(\mathbf{b},\lambda)]^2 = 1$, i.e. the square of any spin is 1. The maximum value of any average P is +1, and the minimum -1. So, for the product of the two spin averages in the integrand,

$$-1 \leq \Psi_e(\mathbf{b},\lambda)\Psi_e(\mathbf{c},\lambda) \leq +1 \tag{14}$$

And since the probability distribution $\rho(\lambda)$ must satisfy

$$\int \rho(\lambda)\mathrm{d}\lambda = 1 \tag{15}$$

then it follows that the second term in the integrand of Eq. (13) helps satisfy

$$\rho(\lambda)[1 - \Psi_e(\mathbf{b}, \lambda)\Psi_e(\mathbf{c}, \lambda)] \geq 0 \tag{16}$$

Referring back to Eq. (14), if we take the absolute value of Eq. (13)

$$|P(\mathbf{a}, \mathbf{b}) - P(\mathbf{a}, \mathbf{c})| \leq \int \rho(\lambda)[1 - \Psi_e(\mathbf{b}, \lambda)\Psi_e(\mathbf{c}, \lambda)]\mathrm{d}\lambda \tag{17}$$

This is just one step away from the famous Bell inequality:

$$|P(\mathbf{a}, \mathbf{b}) - P(\mathbf{a}, \mathbf{c})| \leq 1 + P(\mathbf{b}, \mathbf{c}) \tag{18}$$

Thus, as Bell has assumed a quite general local hidden variable theory, a quantum system that violates this inequality would prove the incompatibility of quantum mechanics and any local hidden variable theory.

2.5 Violations of Bell's Inequality

Bell's paper provided an inequality by which quantum systems could be measured. Experimental proof of violation of this inequalities would show that quantum mechanics is incompatible with local hidden variable theories.

It is interesting to investigate what experimental parameters must be satisfied to achieve a violation of the Bell inequality for a perfect EPR pair. Let's align the $\mathbf{a}$ detector along the $\hat{\mathbf{z}}$ axis, and set the $\mathbf{b}$ and $\mathbf{c}$ detectors to have the same azimuthal angle. If the $\mathbf{b}$ detector is closer to the $\mathbf{a}$ detector, then it must be that $\theta_\mathrm{b} < \theta_\mathrm{c}$, in which the subscript denotes the polar angle to the vector. Noting that Eq. (9) gives us the resultant measurements from each detector based on the angle between them, we can rewrite Bell's inequality as

$$\cos(\theta_\mathrm{b}) - \cos(\theta_\mathrm{c}) \leq 1 - \cos(\theta_\mathrm{c} - \theta_\mathrm{b}) \tag{19}$$

Using trigonometric identities to rewrite $\cos(\theta_\mathrm{c} - \theta_\mathrm{b})$,

$$\cos(\theta_\mathrm{b}) - \cos(\theta_\mathrm{c}) + [\cos(\theta_\mathrm{b})\cos(\theta_\mathrm{c}) + \sin(\theta_\mathrm{b})\sin(\theta_\mathrm{c})] \leq 1 \tag{20}$$

Bell's inequality is therefore maximally violated when the left hand side of Eq. (20) reaches a maximum. Setting the derivative with respect to θ_b equal to zero, we find that $\theta_\mathrm{c} = 2\theta_\mathrm{b}$ for maximum violation. This further simplifies Bell's inequality to

$$2\cos(\theta_\mathrm{b}) - \cos(2\theta_\mathrm{b}) \leq 1 \tag{21}$$

To maximize the violation of Eq. (21) requires that $\theta_\mathrm{b} = 60°$. The ideal experimental setup is therefore to align the detectors at $60°$ and $120°$ angles from the first detector. This gives a maximal violation of $1.5 \leq 1$.

2.6 CHSH Inequality

Bell's inequality and the above theoretical derivations of an experimental setup, however, are not used in practice. Bell's proof "assumed perfect correlations exhibited by the singlet state. However, in real experiments such correlations are practically impossible" [4]. Instead, the group of John Clauser, Michael Horne, Abner Shimony, and Richard Holt built upon Bell's work to rederive an inequality which "provides a way of experimentally testing the local hidden variable model as an independent hypothesis separated from the quantum formalism" [4]. By not assuming the antisymmetric pairing of an EPR state (8), the equality holds for a large class of systems. The resultant CHSH inequality [5] was published in 1969. The inequality is a relation between the expectation values of correlated measurements,

$$|E(\mathbf{a},\mathbf{b}) + E(\mathbf{a}',\mathbf{b}) + E(\mathbf{a},\mathbf{b}') - E(\mathbf{a}',\mathbf{b}')| \leq 2 \tag{22}$$

Here the first particle is measured along one of two axes, $\mathbf{a}$ and $\mathbf{a}'$, for any given trial. In the same trial, the second particle will be measured along either $\mathbf{b}$ or $\mathbf{b}'$. Each E is therefore a correlation of the measurements of the two particles. Experimental verification requires four tests, one for each of the correlation terms in the inequality.

Taking an approach identical to that in Section 2.5, we will derive the theoretically maximal violation of the CHSH inequality for an EPR pair. This is obtained by assuming an azimuthal symmetry of the four possible measurement angles and a polar symmetry such that $\theta_a = \theta_b$ and $\theta_{a'} = \theta_{b'}$, for all angles from the z axis. In the most general case, we assume the orientations of the four apparatuses must be independent of one another. This is diagrammed in Figure (1).

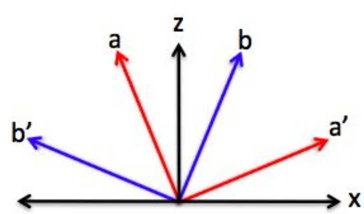

Figure 1: Diagram of optimal angle distribution for CHSH test experiments. Red vectors (a) denote the spin measurement apparatus for the first particle, blue (b) for the second. Calculations show that the angle between each apparatus should be be 45° for maximal violation of the CHSH inequality.

The CHSH inequality can then be written as

$$\cos(\theta_a + \theta_b) + \cos(\theta_a' - \theta_b) + \cos(\theta_b' - \theta_a) - \cos(\theta_a' + \theta_b') =\leq 2 \tag{23}$$

Taking derivatives with respect to both angles, the inequality is maximally violated for the detectors at angles $\theta_a = \theta_b = 22.5°$ and $\theta_a' = \theta_b = 67.5'$. This results in an setup distribution in which the detectors are at 45° to one another. This gives the inequality violation $2\sqrt{2} \leq 2$. Here we have reproduced the Cirel'son inequality [6] by purely geometrical means; it shall be explored in depth in Section 4.3.

In practice, the systems measured were not particle spins, as Bell and EPR had originally considered, but the polarization of photons emitted in an atomic cascade of calcium. This approach was first used by Stuart Freedman and John Clauser in 1971 [7], however it was Aspect, et. al. "who first performed a convincing test of violation of Bell inequalities" [4]. From 1981-2, Alain Aspect led three experiments ([8], [9], [10]) that have become the most famous experimental violations of Bell's theorem. Note that the angle distribution calculated above is different than those used by Aspect, et. al in [8]. This is because of the difference in angle rotation for orthogonal states of photon polarization vs. particle spin.

2.7 Implications of Bell Inequalities

The demise of local hidden variable theories refuted EPR's realist position. Returning to the EPR pair of Eq. (5), it must be that the two particles are entangled.

It is tempting to say that the measurement of, say, the electron *causes* the positron to be in a definite spin. This is not the case. For if it were, entanglement would be a casual influence propagating faster than the speed of light, a relativistic impossibility. As noted by Griffiths, "according to special relativity, there exist inertial frames in which such a signal propagates *backward in time*...and this leads to inescapable logical anomalies" [11]. Instead, consider that we measure the spin of the positron after measuring the spin of the electron. There are reference frames for which the positron measurement occurs first; regardless, spins of the two particles will remain correlated. Thus we consider entanglement to be a superluminal correlation of two subsystems that arises from the initial entanglement, which propagated *sub*luminally. If we consider entanglement to be a fundamental aspect of the bipartite system, the wave function of this system cannot, of course, propagate faster than the speed of light.

Still, such an interaction proves that *Nature is fundamentally nonlocal.* Amazingly, while the interaction of matter is local (systems must be in contact to become initially entangled), the effects of interaction last even after the separation of matter in space and time. We can no longer describe most systems with local quantum states; instead, the wave function links and spreads over all the subsystems. This suggests the difficulty of achieving truly isolated systems. Such a discovery is one of the most philosophically beautiful accomplishments in quantum theory.

3 Density Matrices

3.1 Pure States

To delve further requires the use of density matrices as a mathematical tool. Density matrices allow us to encapsulate knowledge of entanglement between systems. They also make clear the distinction between pure and mixed states of a system.

As described in Section 2.2, a pure state is the wave function of a quantum system for which we possess complete information. In contrast, a mixed state is a probabilistic sum of pure states. A mixed state can be said to be a system for which we do not possess complete information; as it is a sum of pure states, the probabilities represent our incomplete knowledge as to *which* of the pure states the system is actually in. It is important to keep in mind the distinction between the classical probabilities p in mixed states and the square-integrable coefficients $c = \sqrt{p}$ of a superposition of basis states.

The density matrix ρ for a general state (2) is simply the projection operator on that state, which is the tensor product of the state with itself

$$\rho = |\psi\rangle \langle\psi| = \sum_{ij} c_i c_j^* |\psi_i\rangle \langle\psi_j| \tag{24}$$

The diagonal terms correspond to $c_i c_i^* |\psi_i\rangle \langle\psi_i|$, the projection onto that basis state. This gives the probability of the system being in basis state $|\psi_i\rangle$. The off-diagonal terms are non-zero only when $|\psi\rangle$ is a linear superposition of the basis vectors, and therefore capture the coherence, or interference, between the components $|\psi_i\rangle$.

Reintroducing the general product state given in Eq. (4), $|\psi\rangle = |\alpha\rangle_1 |\beta\rangle_2$, we see that the density matrix in Eq. (24) simplifies to

$$\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i| = \sum_i p_i |\alpha_i\rangle_1 |\beta_i\rangle_2 \langle\beta_i|_2 \langle\alpha_i|_1 \tag{25}$$

Product states are factorizable, and are thus pure states without entanglement between the two subsystem $|\alpha\rangle_1$ and $|\beta\rangle_2$. Here, i serves as the "hidden variable," giving us complete information of the system. Such a system will not violate any of the Bell Inequalities. Eq. (25) shows that there is no coherence between the set of basis vectors that diagonalizes the density matrix.

It is important to stress that entanglement occurs between *components* of a system or subsystems. These components each have their own Hilbert space. There will always be a basis "in which the density matrix becomes diagonal...thus our association between"[[12]] interference and entanglement is not absolute. Pure states may or may not contain entanglement among the components of the system.

Our Bell state of the EPR pair in Eq. (5) has so far provided an excellent example of a pure state showing entanglement between two subsystems. Rewriting Eq. (5) in more mathematically obvious terms, our basis for the bipartite system is given in Eq. (4) as

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \uparrow_+\uparrow_- \quad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \uparrow_+\downarrow_- \quad \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \downarrow_-\uparrow_- \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \downarrow_+\downarrow_- \tag{26}$$

and therefore we can express the EPR pair by the density matrix

$$\rho_{\text{Bell}} = \frac{1}{2}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 & 1 & -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{27}$$

The off-diagonal terms $(-\frac{1}{2})$ describe the coherence between the states $\uparrow_1\downarrow_2$ and $\downarrow_1\uparrow_2$, in which both subsystems change state. In this case, the coherence between states is due to entanglement. As an example of coherence that is not due to entanglement, were the density matrix to read

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \gamma & 0 & 0 \end{pmatrix} \tag{28}$$

the γ term would represent coherence between the states $\downarrow_1\downarrow_2$ and $\uparrow_1\downarrow_2$. As the state of the second particle does not change, this is only coherence within the first particle, and thus does not capture entanglement. This is a mathematical example of entanglement being a special case of coherence or interference.

Furthermore, it is worth showing how to write our Bell state as a product state. Choosing our basis to be the singlet and triplet states of a bipartite system,

$$\rho_{\text{Bell}} = \begin{array}{r} S=0 \\ S=1, S_z=+1 \\ S=1, S_z=0 \\ S=1, S_z=-1 \end{array} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{29}$$

Our matrix contains only one element because the EPR is fully described by the singlet state. Yet we have seen in Eq. (27) that within the singlet state there is coherence and entanglement. This hints at the ability of density matrices to accommodate quantum information at any scale. No matter how complex a subsystem is, it is always possible to consider the subsystem in it's entirety in relation to other subsystems in a relatively simple manner.

3.2 Mixed States

In our Bell State example, we have knowledge of both the electron and positron. This allows us to write their composite wave function as a pure state. However, what if we look at just the electron? To describe the electron, we must refer back to the basis give in Eq. (1). The pure states are $\uparrow$ and $\downarrow$, and we find that the electron is in each state with equal (classical) probability, $p_\uparrow = p_\downarrow = \frac{1}{2}$. Thus we must describe the system using these classical probabilities. Accordingly, the mixed state density matrix is given by

$$\rho_{\text{mixed}} = \sum_i p_i \rho_i = \frac{1}{2}\left|\uparrow\right\rangle\left\langle\uparrow\right| + \frac{1}{2}\left|\downarrow\right\rangle\left\langle\downarrow\right| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \tag{30}$$

The entanglement between electron and positron still exists physically, but it is impossible to observe if we only look at the electron. The pure states that compose a mixed state may contain nontrivial quantum superposition and entanglement, but there is no entanglement *between* these basis states. Put philosophically, the whole of a quantum system is more than just the sum of its parts.

Let's modify our EPR experiment to introduce classical noise, which may be handled by a mixed-state density matrix. Suppose that our EPR pair is generated not by muon decay, but by a black box. This device creates a fully entangled EPR pair with probability f. The rest of the time, the particles come out with random, but definite, spins. In the classical case, our density matrix is simply a statistical mixture of the probability of being in a given spin state for each particle:

$$\rho_{\text{classical}} = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix} \tag{31}$$

By taking into account the performance of the black box, we can account for both scenarios:

$$\rho = f \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + (1-f) \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix} \tag{32}$$

This is a generalized Werner state [13], $\rho_w = f\rho_{\text{Bell}} + \frac{1}{4}(1-f)\mathbb{I}$.

4 Fidelity of Bell Test Experiments

Having introduced density matrices as a tool for determining entanglement, we can investigate the fidelity of experiments looking to violate Bell inequalities and LHVM. The Werner state give an accurate depiction of an experimental setup for a single channel Bell test experiment. As with any experimental setup, a certain amount of data will be noise, or something unexpected. By varying the parameter f, we can set limits on the fidelity of an experimental setup to violate Bell's inequality and the CHSH inequality for the optimal angle distributions found in Sections 2.5 and 2.6, respectively. While it is intuitive that we may use a modification of Eq. (19),

$$f\left(\cos(\theta_{\text{b}}) - \cos(\theta_{\text{c}}) + \cos(\theta_{\text{c}} - \theta_{\text{b}})\right) \leq 1 \tag{33}$$

to find the minimum fidelity of a generalized Werner state in violation of LHVM, for more complicated systems it is advantageous to deal with density matrices. We will use these calculations to demonstrate the effectiveness of the density matrix formalism.

4.1 Trace Operation

This will require extracting information from the density matrices of each quantum system. Observables are derived from density matrices via trace operations with an operator. The trace operation is mathematically defined as

$$\mathrm{Tr}(\hat{A}) \equiv \sum_i \langle \phi_i | \hat{A} | \phi_i \rangle \tag{34}$$

for an orthonormal basis $\{|\phi_i\rangle\}$. Any pure or mixed state must be normalized by $|\langle \psi | \psi \rangle|^2 = 1$; this condition can be reformulated as

$$\mathrm{Tr}(\rho) = 1 \tag{35}$$

If we consider the identity matrix as an operator, then the trace rule gives us the expectation value of the observable, $\mathrm{Tr}(\rho\mathbb{I}) = \langle \mathbb{I} \rangle = 1$. This relation also holds for a general operator $\hat{A}$ with eigenstates $|a_i\rangle$ and corresponding eigenvalues a_i, the trace rule gives

$$\mathrm{Tr}(\rho\hat{A}) = \sum_i \langle a_i | (|\psi\rangle \langle \psi|) \hat{A} | a_i \rangle = \sum_i a_i | \langle a_i | \psi \rangle |^2 \tag{36}$$

The term $|\langle a_i | \psi \rangle|^2$ is the Born probability that the measurement $\hat{A}$ will yield the value a_i. The summation then, as Schlosshauer notes, is the expectation value $\left\langle \hat{A} \right\rangle$: "an average over all possible outcomes...weighted by the corresponding Born probabilities" [12].

4.2 Fidelity of Bell Inequality Tests

Using the trace operation, we can utilize our Werner mixed density matrix to determine the experimental fidelity needed to violate the Bell inequality give in Eq. (18). For the optimal angle distribution we set **a** along the $\hat{\mathbf{z}}$ axis, therefore the corresponding Pauli spin operator is σ_z. The measuring apparatus **b** has a polar angle of 60°, so it's operator is calculated trigonometrically to be

$$\hat{\mathbf{b}} = \cos(60^\circ)\sigma_z + \sin(60^\circ)\sigma_x = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \tag{37}$$

Similarly, the second polar angle of 120° gives

$$\hat{\mathbf{c}} = \cos(120^\circ)\sigma_z + \sin(120^\circ)\sigma_x = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \tag{38}$$

in which we have chosen the azimuthal angle to be 0° in accordance with the assumptions made in Section 2.5.

Bell's derivation assumes a perfect singlet configuration, allowing $P(\mathbf{a}, \mathbf{b})$ in Eq. (11) to be written as an integral over only the electron wave function. For our Werner state, classical noise prohibits us from making the same assumption. We therefore construct our operator $P(\mathbf{a}, \mathbf{b})$ as measuring the spin of the electron along $\mathbf{a}$ and the spin of the positron along $\mathbf{b}$:

$$\hat{P}_{ab} = \hat{a} \otimes \hat{b} = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \tag{39}$$

Using the trace operation, we can act on the density matrix for the Werner state

$$P(\mathbf{a}, \mathbf{b}) = \mathrm{Tr}\left[\rho_w \hat{P}_{ab}\right] \tag{40}$$

$$= \mathrm{Tr}\left[\begin{pmatrix} \frac{1}{4}(1-f) & 0 & 0 & 0 \\ 0 & \frac{1}{4}(1+f) & -\frac{1}{2}f & 0 \\ 0 & -\frac{1}{2}f & \frac{1}{4}(1+f) & 0 \\ 0 & 0 & 0 & \frac{1}{4}(1-f) \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}\right] \tag{41}$$

Simplification results in $P(\mathbf{a}, \mathbf{b}) = \frac{1}{2}f$. Similar trace operations yield $P(\mathbf{a}, \mathbf{c}) = P(\mathbf{b}, \mathbf{c}) = -\frac{1}{2}f$. The Bell inequality (18) can now be rewritten in terms of the fidelity of the experimental setup,

$$\frac{3}{2}f \leq 1 \tag{42}$$

An EPR pair setup therefore requires a fidelity of $f > \frac{2}{3}$ to achieve an experimental violation of the Bell inequality. For $f < \frac{2}{3}$, it is impossible to conclude that quantum mechanics is incompatible with LHVM or that the quantum system under consideration contains entangled spins.

4.3 Fidelity of CHSH Inequality Tests

A similar approach is used to determine the fidelity of CHSH inequality test experiments. Correlation functions are determined by trace operations with operators of the given spins acting on the quantum state,

$$E(\mathbf{a}, \mathbf{b}) = \mathrm{Tr}(\rho_W(\sigma_{1\mathbf{a}} \otimes \sigma_{2\mathbf{b}})) \tag{43}$$

While the CHSH inequality (22) is broadly defined, so that we may compare with Section 4.2 we choose the same experimental setup. The two particles are that of the EPR pair, and due to experimental fidelity the density matrix is ρ_w.

Using the optimal angle distribution from Section 2.6, we set $\mathbf{a}$ on the $\hat{\mathbf{z}}$ axis for ease calculation. Then $\mathbf{b}$ is 45° from the polar axis, such that

$$\sigma_{2\mathbf{b}} = \frac{\sqrt{2}}{2}\sigma_z + \frac{\sqrt{2}}{2}\sigma_x = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{44}$$

This gives the operator

$$\sigma_{1\mathbf{a}} \otimes \sigma_{2\mathbf{b}} = \frac{\sqrt{2}}{2} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix} \tag{45}$$

which is used to determine the first correlation function

$$E(\mathbf{a},\mathbf{b}) = \mathrm{Tr}\left[\frac{\sqrt{2}}{2} \begin{pmatrix} \frac{1}{4}(1-f) & 0 & 0 & 0 \\ 0 & \frac{1}{4}(1+f) & -\frac{1}{2}f & 0 \\ 0 & -\frac{1}{2}f & \frac{1}{4}(1+f) & 0 \\ 0 & 0 & 0 & \frac{1}{4}(1-f) \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix} \right] \tag{46}$$

$$= \frac{\sqrt{2}}{2} f \tag{47}$$

The other correlation functions are computed to be $E(\mathbf{a}',\mathbf{b}) = E(\mathbf{a},\mathbf{b}') = \frac{\sqrt{2}}{2}f$ and $E(\mathbf{a}',\mathbf{b}') = -\frac{\sqrt{2}}{2}f$. The allows us to rewrite the CHSH inequality in terms of the fidelity,

$$2\sqrt{2}f \leq 2 \tag{48}$$

Thus $f > \frac{\sqrt{2}}{2} = 0.7071$ allows for an experimental verification of Bell's theorem and shows the incompatibility of LHVM and quantum mechanics.

4.4 Mathematical Limits of Entanglement

It is interesting to note that a Werner state of $f = \frac{1}{3}$ produces a density matrix for which it is impossible to mathematically conclude that the system contains entanglement.

$$\rho_{f=1/3} = \begin{pmatrix} \frac{1}{6} & 0 & 0 & 0 \\ 0 & \frac{1}{3} & -\frac{1}{6} & 0 \\ 0 & -\frac{1}{6} & \frac{1}{3} & 0 \\ 0 & 0 & 0 & \frac{1}{6} \end{pmatrix} \tag{49}$$

This density matrix is the same for the state

$$\frac{1}{6}(\uparrow_1\downarrow_2 + \uparrow_2\downarrow_1 + \rightarrow_1\leftarrow_2 + \leftarrow_1\rightarrow_2 + \otimes_1 \odot_2 + \odot_1\otimes_2) \tag{50}$$

written in the same spin basis as the Werner state. Here, spins along the z, x, and y axes are described by vertical arrows, horizontal arrows, and arrows perpendicular to the page, respectively. By convention, systems are only considered to have entanglement if it is impossible to write their states in a manner such that the subsystems are in no manner entangled. As such, an observer presented with the matrix (49), or a similar Werner state matrix for $f < \frac{1}{3}$, must mathematically conclude that the system contains no entanglement between the spin components. This statement does not relate the

Bell inequalities or the incompatibility of quantum mechanics with LHVM. It is an independent calculation in which we show how the choice of basis in evaluating density matrices sets a limit on the our knowledge of the entanglement of a system.

5 Entropy of Entangled Systems

5.1 von Neumann Entropy

As physicists, it is important to be able to quantify the entanglement of a system. Such a quantification can be found using density matrices, most commonly by calculating the von Neumann entropy [14],

$$S(\rho) \equiv -\mathrm{Tr}(\rho \log_2 \rho) \tag{51}$$

or, equivalently, a sum over the eigenvectors λ of the density matrix,

$$S(\rho) \equiv -\sum_i \lambda_i \log_2 \lambda_i \tag{52}$$

As Schlosshauer notes, "the von Neumann entropy can be viewed as a generalization of the notion of entropy in classical statistical mechanics" [12]. In statistical mechanics, the entropy of a system characterizes the number of possible states the system available to the system. It is a measure of our knowledge, or ignorance, of the system. Appropriately, the von Neumann entropy characterizes the "degree of 'mixedness'" [12] of the density matrix. A quantum system with a high degree of mixedness may be in any number of pure states, and will have high entropy. A quantum system for which we have complete information (i.e. is in a pure state) has zero entropy. We have already established that our Bell state in Eq. (5) is a pure state. To confirm it's von Neumann entropy, the eigenvalues of ρ_{Bell} are 1, 0, 0, & 0, therefore:

$$S(\rho_{\mathrm{Bell}}) = -\left[1\log_2 1 + 3(0\log_2 0)\right] = 0 \tag{53}$$

By convention, $0\log_2 0 = 0$. Conceptually, it is reasonable to consider the Bell state to have zero entropy: both particles are in a single, composite state because they are maximally entangled.

The maximum von Neumann entropy of a system can be found be considering a completely mixed state. Using Eq. (31), we know that a fully mixed state has each component of the system in each basis state with equal probability, and is thus proportional to the identity matrix $\mathbb{I}$. Generalizing to an arbitrarily high dimensionality $\mathbb{C}^N$,

$$\rho_{\mathrm{mixed}} = \frac{1}{N}\mathbb{I} \tag{54}$$

will have N eigenvalues, $\lambda_i = p_i = 1/N$. The von Neumann entropy of a maximally mixed state is therefore,

$$S(\rho_{\text{mixed}}) = -\sum_{i}^{N} \frac{1}{N} \log_2 \frac{1}{N} = \log_2 N \tag{55}$$

Let's look at the particles in our EPR pair separately. We found in Eq. (30) that $\rho_+ = \rho_- = \frac{1}{2}\mathbb{I}$ in $\mathbb{C}^2$. As such, von Neumann entropy of the individual particles is maximal: $S_+ = S_- = \log_2 2 = 1$. How, then, is the entropy of the composite system (both particles together in an EPR pair), equal to zero?

In quantum mechanics, the von Neumann entropy of a composite system can be less than the von Neumann entropy of it's subsystems because the subsystems may be entangled. In this case, the spins of the positron and electron are entangled with one another, and the von Neumann entropy of one spin is "canceled" by being correlated with the von Neumann entropy of the second spin. This inequality of subadditivity for entangled subsystems was proven in 1970 by Huzihiro Araki and Elliot Lieb [15]:

$$S\rho_{\text{AB}} \leq S\rho_{\text{A}} + S\rho_{\text{B}} \tag{56}$$

in which the von Neumann entropies are additive only if the two systems are separable, $S(\rho_{\text{AB}}) = S(\rho_{\text{A}} \otimes \rho_{\text{B}})$.

5.2 Purity

There are other interesting methods by which to measure the entanglement of a system. Schlosshauer explains the purity of a density matrix, a "simple and commonly used measure" [12] of the degree of mixedness of a system. Since a density matrix is the projection operator of the basis states onto themselves, it must be that

$$\rho^2 = \sum_{ij} p_i p_j \left|\psi_i\right\rangle \left\langle\psi_j\right| \left\langle\psi_i\right| \left|\psi_i\right\rangle \tag{57}$$

A pure state density matrix will yield

$$\rho^2 = \sum_{i} p_i \left|\psi_i\right\rangle \left\langle\psi_i\right| = \rho^2 \tag{58}$$

whereas a mixed density matrix, even if written in a basis for which there are no off-diagonal terms, yields

$$\rho^2 = \sum_{i} p_i^2 \left|\psi_i\right\rangle \left\langle\psi_i\right| \neq \rho^2 \tag{59}$$

Using this, the purity of a system is defined as,

$$\mu \equiv \text{Tr}(\rho^2) \tag{60}$$

The trace of a pure state density matrix is always 1, as it must satisfy the normalization condition $\sum_{ij}$, the coefficients of the basis states as given in Eq. (2). For a mixed state, μ is determined by the probabilities seen in Eq. (59),

$$\mu = \sum_{i=1}^{N} p_i^2 \tag{61}$$

As a maximally mixed system is given by Eq. (54), the minimum purity of a system is

$$\mu_{\min} = \sum_{i=1}^{N} \frac{1}{N^2} = \frac{1}{N} \tag{62}$$

6 Entanglement With the Environment

With an understanding of the entropic effects of entanglement, it is useful to consider placing a quantum system into a non-isolated environment. We can use our EPR pair in an argument modified from [12]. Consider that our muon decay creates an electron-positron pair in vacuum. This, as always, is given by the Bell state. As the particles fly apart, they will exit the vacuum and be bombarded by environmental photons, air molecules, background radiation, etc. While we may not know the exact composition of the environment, we can describe all the subsystems of the environment as a single composite wave function.

Before this system-environment interaction, both systems may be described as a product state,

$$|\psi\rangle |E_0\rangle = \frac{1}{\sqrt{2}}(|{\uparrow_1\downarrow_2}\rangle - |{\downarrow_1\uparrow_2}\rangle) |E_0\rangle \tag{63}$$

Depending on the state of the EPR system, these environmental particles will scatter in different manners, changing $|E_0\rangle$. For the sake of this example, we make the simplifying assumption that the environment only become coupled with the **z** spins of EPR pair. We notate the evolution as

$$|{\uparrow_1\downarrow_2}\rangle |E_0\rangle \to |{\uparrow_1\downarrow_2}\rangle |E_1\rangle \tag{64}$$

$$|{\downarrow_1\uparrow_2}\rangle |E_0\rangle \to |{\downarrow_1\uparrow_2}\rangle |E_2\rangle \tag{65}$$

As the system evolves, the relative states of the EPR system become entangled with the environmental states,

$$\frac{1}{\sqrt{2}}(|{\uparrow_1\downarrow_2}\rangle - |{\downarrow_1\uparrow_2}\rangle) |E_0\rangle \to \frac{1}{\sqrt{2}}(|{\uparrow_1\downarrow_2}\rangle |E_1\rangle - |{\downarrow_1\uparrow_2}\rangle |E_2\rangle) \tag{66}$$

This shows the spread of the superposition between components of the EPR subsystem to a shared superposition between components of the composite system-environment state. In effect, the EPR pair has become entangled with the environment, ensuring that coherence "is no longer a property of the [sub]system alone: it has become a shared property of the global system-environment state" [12]. Entanglement has delocalized the coherence over a greater number of degrees of freedom. For the observer who only has access to the EPR subsystem, this coherence appears to be irretrievably lost. In terms of entropy, the entanglement of the EPR pair with the environment causes the states of the two subsystems to no longer be separable. By the inequality of subadditivity (56), it must be that this interaction has decreased the overall von Neumann entropy. As the von Neumann entropy of a minimally mixed state is zero, "environmental monitoring" is a thermodynamic quantifier of information: increasing entangled interactions increasingly draws information from the subsystem in question. For the observer who only focuses on the EPR pair, it's superposition appears to have been lost. This is the meaning of entanglement as the entropic force between the decoherence of a quantum-to-classical transition.

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