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Demystifying decoherence and the master equation of quantum Brownian motion

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Quantum decoherence is a proposed mechanism for the emergence of classical physics from the quantum mechanics. It has been developed extensively in recent years, but is sufficiently technically complicated to discourage widespread understanding. In this paper we provide a gentle introduction to quantum decoherence. We introduce state operators and their density matrix representations to describe composite systems, such as an experiment and its environment. We illustrate how the loss of information about a subsystem can cause a quantum system to appear classical. We first analyze a discrete example of phase randomization, then a Bell state, and finally a continuous system. In the final case we provide an accessible derivation of a major early result of decoherence theory, the master equation of quantum Brownian motion. We conclude by applying the master equation to the decoherence of a simple harmonic oscillator, with results reminiscent of our earlier discrete examples. © 2009 American Association of Physics Teachers. [DOI: 10.1119/1.3043847]

I. INTRODUCTION

Decoherence theory gives a profound window into quantum mechanics by making the connection between physics and information not just clear, but necessary.¹ Informally, decoherence describes the emergence of classical behavior from quantum mechanics by information leakage; if the quantum-specific details of a system “leak” outside our measurement capability, we cannot observe them. The details of decoherence theory are sufficiently complicated to discourage students and physicists from other fields to pursue a basic understanding of decoherence. The available literature is aimed at an advanced audience and contains significant gaps for most physicists.²⁻⁶

In this paper we attempt to rectify this situation by making the underlying concepts associated with decoherence accessible to a more general audience. We begin in Sec. II by introducing the concept of a state operator, an object of central importance to quantum decoherence theory, through a simple example first developed by Bernstein.⁷ We consider a rudimentary universe consisting of quantum particles and an “environment” randomized by a roulette wheel, and show that this randomization leads to diagonalization of the state operator and the emergence of classical behavior.

In Sec. III we put the treatment in Sec. II on a firmer mathematical foundation by an example involving an entangled pair of particles. We show that restricting ourselves to knowledge of only one particle in the pair through a partial trace has the same effect as the phase randomization process employed in Sec. II.⁸ Following Halliwell, in Sec. IV we develop a simple master equation for decoherence in a continuous model of quantum Brownian motion.³ In Sec. V we show that, with reasonable assumptions, the master equation found in Sec. IV results in the same phenomena as we saw in the simple examples of Secs. II and III.⁹ Finally, we demonstrate how the master equation results in the decoherence of a quantum simple harmonic oscillator in a thermal bath.⁶

II. THE STATE OPERATOR AND PHASE RANDOMIZATION

A. State operator

To begin, we consider the simplest possible case: spin one-half particles. In particular, we consider spin one-half neutral silver atoms, each of which has one unpaired electron. The spin operator \hat{S} represents each atom’s spin angular momentum in a two-dimensional Hilbert space. \hat{S} obeys the well-known commutation relations¹⁰⁻¹²

$$i\hbar\hat{S}_x = \hat{S}_y\hat{S}_z - \hat{S}_z\hat{S}_y, \quad (1a)$$

$$i\hbar\hat{S}_y = \hat{S}_z\hat{S}_x - \hat{S}_x\hat{S}_z, \quad (1b)$$

$$i\hbar\hat{S}_z = \hat{S}_x\hat{S}_y - \hat{S}_y\hat{S}_x, \quad (1c)$$

and has the matrix representation

$$\hat{S}_x = \frac{\hbar}{2}\hat{\sigma}_x, \quad \hat{S}_y = \frac{\hbar}{2}\hat{\sigma}_y, \quad \hat{S}_z = \frac{\hbar}{2}\hat{\sigma}_z, \quad (2)$$

where

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (3)$$

are the familiar Pauli matrices.⁸ These operators and the identity \hat{I} form a complete basis for operators in Hilbert space. That is,

$$\hat{A} = r_I\hat{I} + \frac{r_x}{2}\hat{\sigma}_x + \frac{r_y}{2}\hat{\sigma}_y + \frac{r_z}{2}\hat{\sigma}_z = \frac{1}{2} \begin{pmatrix} 2r_I + r_z & r_x - ir_y \\ r_x + ir_y & 2r_I - r_z \end{pmatrix}, \quad (4)$$

where \hat{A} is an arbitrary operator, the factors of 2 are by convention, and r_I , r_x , r_y , and r_z are complex scalars.⁸

We may write the state vector for any spin state of a silver atom as

$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle = \alpha\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta\begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (5)$$

a superposition of spin-up and spin-down, defined conventionally as the eigenstates of \hat{S}_z . Because $|\psi\rangle$ is normalized, its magnitude is unity;

$$\langle\psi|\psi\rangle = (\alpha^* \ \beta^*)\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha\alpha^* + \beta\beta^* = 1. \quad (6)$$

We construct the state operator and corresponding (density) matrix representation¹³ by forming the outer product^{12,14}

$$\hat{\rho} = |\psi\rangle\langle\psi| = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}(\alpha^* \ \beta^*) = \begin{pmatrix} \alpha\alpha^* & \alpha\beta^* \\ \beta\alpha^* & \beta\beta^* \end{pmatrix}. \quad (7)$$

Although the state vector $|\psi\rangle$ is physically equivalent to $e^{i\phi}|\psi\rangle$ for any real ϕ , the state operator is free from this ambiguity and is unique for any state. By Eqs. (6) and (7) the trace of $\hat{\rho}$ is unity,

$$\text{Tr}(\hat{\rho}) = \alpha\alpha^* + \beta\beta^* = 1. \quad (8)$$

Because $\hat{\rho}$ is an operator, we can represent it by Eq. (4), so Eq. (8) becomes

$$\text{Tr}(\hat{\rho}) = \frac{1}{2}(2r_I + r_z + 2r_I - r_z) = 2r_I = 1, \quad (9)$$

which implies that $r_I = 1/2$.⁸ Equation (7) shows that $\hat{\rho}$ is a Hermitian operator,

$$\hat{\rho}^\dagger = (|\psi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\psi| = \hat{\rho}. \quad (10)$$

Hence, r_x , r_y , and r_z are real, and $\hat{\rho}$ is a projection operator,¹⁰

$$\hat{\rho}^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = \hat{\rho}, \quad (11)$$

so $r_x^2 + r_y^2 + r_z^2 = 1$. We may represent each of the components of the unit vector \vec{r} in spherical coordinates as⁸

$$r_x = \sin \theta \cos \phi, \quad (12a)$$

$$r_y = \sin \theta \sin \phi, \quad (12b)$$

$$r_z = \cos \theta. \quad (12c)$$

B. Phase randomizer

With this machinery in hand, we next consider a thought experiment. Suppose that a silver furnace is connected to an angular control device, which polarizes the spin of outgoing atoms in the $\theta = \pi/2$, x - y plane at an user-specified angle ϕ .⁷ Hence, we write Eq. (12) as

$$r_x = \cos \phi, \quad (13a)$$

$$r_y = \sin \phi, \quad (13b)$$

$$r_z = 0. \quad (13c)$$

By Eq. (4), the state operator of the atom has the matrix representation

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} 1 + 0 & \cos \phi - i \sin \phi \\ \cos \phi + i \sin \phi & 1 - 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix}. \quad (14)$$

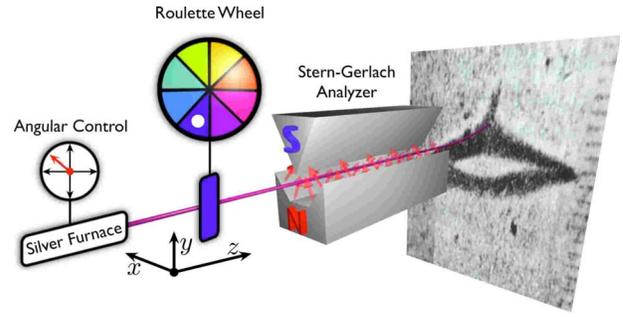


Fig. 1. (Color online) A Stern-Gerlach apparatus sorts atoms either up or down, depending on their spin. We insert a roulette wheel between the angular control and the Stern-Gerlach apparatus to crudely model an external environment. Each time an atom passes the roulette wheel, we spin the roulette wheel and add a random value between 0 and 2π to the atom's original spin angle, ϕ (Ref. 15).

We next place a Stern-Gerlach analyzer along the path of the silver beam to measure the spin of the atoms. The analyzer, shown in Fig. 1, consists of an inhomogeneous magnetic field that sorts spin one-half particles into two bands based on their magnetic moments, which are proportional to their spins.⁷ If we place the magnetic field gradient of the analyzer along the $+\hat{y}$ axis, then the spin-sorter observable is

$$\hat{O} = \hat{y} \cdot \hat{S} = \frac{\hbar}{2} \hat{\sigma}_y, \quad (15)$$

and we always observe the eigenvalues $\pm\hbar/2$.

To calculate the observed average value we use the state operator to find the spin expectation value $\langle\hat{O}\rangle$. For any observable \hat{A} we have¹²

$$\begin{aligned} \text{Tr}(\hat{\rho}\hat{A}) &= \sum_i \langle\alpha_i|(|\psi\rangle\langle\psi|\hat{A})|\alpha_i\rangle = \sum_i \langle\psi|\hat{A}|\alpha_i\rangle\langle\alpha_i|\psi\rangle \\ &= \langle\psi|\hat{A}\left(\sum_i |\alpha_i\rangle\langle\alpha_i|\right)|\psi\rangle = \langle\psi|\hat{A}|\psi\rangle = \langle\hat{A}\rangle, \end{aligned} \quad (16)$$

where $\{|\alpha_i\rangle\}$ is any orthonormal, complete basis, so $\sum_i |\alpha_i\rangle\langle\alpha_i| = I$ is the identity. We apply this important result to \hat{O} and obtain

$$\begin{aligned} \langle\hat{O}\rangle &= \text{Tr}(\hat{\rho}\hat{O}) \\ &= \frac{\hbar}{4} \text{Tr} \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ &= \frac{\hbar}{4} (ie^{-i\phi} - ie^{i\phi}) = \frac{\hbar}{2} \sin \phi, \end{aligned} \quad (17)$$

which is plotted in Fig. 2. As we might expect, the apparatus measures how close the silver atoms are aligned with the magnetic field gradient. When $\phi=0$, the atom's spin points along \hat{x} , which is orthogonal to the magnetic field. Hence, half of our measurements yield $+\hbar/2$, while half give $-\hbar/2$, averaging to zero. When $\phi=\pi/2$, the atom spin points along $+\hat{y}$, so we find $+\hbar/2$ every time. Similarly, when $\phi=-\pi/2$, we always measure $-\hbar/2$.⁷ This behavior is characteristic of a coherent quantum superposition and a nondiagonal state operator.

To crudely model the environment we add another component to our apparatus, a classical roulette wheel, between

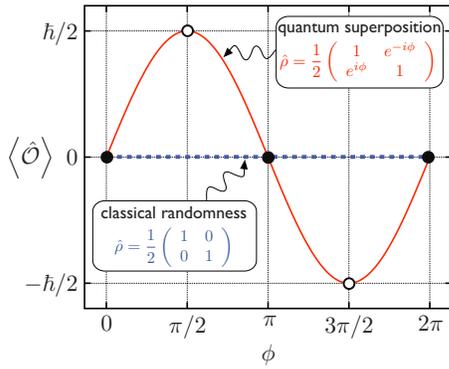


Fig. 2. (Color online) The expectation value of the spin-sorter observable \hat{O} with varying spin angle ϕ . Equation (17), plotted as a solid line, shows the quantum behavior of the original system. The filled circles represent destructive quantum interference, and the open circles denote constructive interference. As indicated in Eq. (19) and shown as a dashed line, the randomness of the roulette wheel destroys the quantum nature of the system.

the angle control device and the Stern-Gerlach analyzer, as shown in Fig. 1. The roulette wheel is continuous and ranges in value between 0 and 2π . Whenever an atom passes by, we spin the roulette wheel and add its value, ϕ_R , to the atom's original spin angle, ϕ . In this way the atom is given a new spin angle, $\phi' = \phi + \phi_R$, which we then measure using the Stern-Gerlach apparatus.⁷ Note that because the atom's spin is periodic in 2π and ϕ_R is random in the interval 2π , ϕ' is a random number between 0 and 2π .

To calculate the expectation value $\langle \hat{O} \rangle_R$ of \hat{O} with the roulette wheel, we first need to find $\hat{\rho}_R$, the new state operator that takes the roulette wheel into account. Because \hat{O} is independent of the roulette wheel angle ϕ , averaging \hat{O} reduces to averaging $\hat{\rho}$. Hence, we proceed by averaging the angle in Eq. (14) over the interval 0 to 2π . We obtain

$$\begin{aligned} \hat{\rho}_R &= \frac{1}{2\pi} \int_0^{2\pi} d\phi' \hat{\rho} \\ &= \frac{1}{2} \begin{pmatrix} \frac{1}{2\pi} \int_0^{2\pi} d\phi' \times 1 & \frac{1}{2\pi} \int_0^{2\pi} d\phi' \times e^{-i\phi'} \\ \frac{1}{2\pi} \int_0^{2\pi} d\phi' \times e^{i\phi'} & \frac{1}{2\pi} \int_0^{2\pi} d\phi' \times 1 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2} \hat{I}. \end{aligned} \quad (18)$$

Now, we use Eqs. (15) and (16) to calculate the expectation value

$$\langle \hat{O} \rangle_R = \text{Tr}(\hat{\rho}_R \hat{O}) = \text{Tr}\left(\frac{1}{2} \hat{I} \frac{\hbar}{2} \hat{\sigma}_y\right) = \frac{\hbar}{4} \text{Tr}(\sigma_y) = 0, \quad (19)$$

which, as required, is independent of the initial choice of ϕ . Now at every angle, rather than just $\phi=0$ or $\phi=\pi$, half our measurements yield $\hbar/2$ and half yield $-\hbar/2$.⁷ This behavior is characteristic of a classical mixture and a diagonal state operator. We plot this result in Fig. 2. This result is expected, because it corresponds to letting ϕ go to ϕ' and averaging the original expectation value $\langle \hat{O} \rangle$ [the right side of Eq. (17)], which also yields an expectation value of zero.

This thought experiment hints at a fundamental difference between the cases without and with the roulette wheel. The randomness of the roulette wheel kicked the spin of the atom a random amount, which effectively destroyed the off-diagonal elements of the state operator in Eq. (14), while leaving the diagonal elements intact. The loss of the off-diagonal terms results in the loss of the sinusoidal pattern, a quantum effect, as we saw in Fig. 2. As we will see, this loss was no accident: the destruction of off-diagonal elements is the hallmark of a loss of quantum information and the emergence of the classical world.^{2,8,9}

Our discussion has been quite abstract so far, and the reader might wonder how such a roulette wheel might work in a physical system. If the initial state of the atom is the superposition in Eq. (5), then under the Schrödinger equation it evolves to

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}(e^{-iE_{\uparrow}t/\hbar}|\uparrow\rangle + e^{-iE_{\downarrow}t/\hbar}|\downarrow\rangle). \quad (20)$$

Because the atom has a magnetic moment $\mu_z = \gamma S_z$, where γ is the gyromagnetic ratio, its interaction energy with an external magnetic field B_z is

$$E = \mu_z B_z = \gamma B_z S_z, \quad (21)$$

where $S_z = \pm \hbar/2$. Hence, the state vector

$$\begin{aligned} |\psi(t)\rangle &= \frac{1}{\sqrt{2}}(e^{-i\gamma B_z t/2}|\uparrow\rangle + e^{+i\gamma B_z t/2}|\downarrow\rangle) \\ &= \frac{1}{\sqrt{2}}e^{-i\gamma B_z t/2}(|\uparrow\rangle + e^{+i\gamma B_z t}|\downarrow\rangle), \end{aligned} \quad (22)$$

and the corresponding state operator has the matrix representation

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)| = \frac{1}{2} \begin{pmatrix} 1 & e^{-i\beta} \\ e^{i\beta} & 1 \end{pmatrix}, \quad (23)$$

where $\beta = \gamma B_z t$. Equation (23) has the same form as Eq. (14). Thus, the roulette wheel can mimic a fluctuating environmental magnetic field. Such fluctuations effectively destroy quantum coherence and are responsible for the emergence of classical behavior.

III. REDUCED STATE OPERATORS AND PARTIAL INFORMATION

In Sec. II we saw how an external device, a roulette wheel, destroyed the off-diagonal elements of the density matrix representation of the state operator. Equivalently, we may view the loss of the off-diagonal elements as a result of only partial knowledge of the total system. That is, in Eq. (18) we focused on the silver atom, while only keeping track of the roulette wheel statistically.⁷ It was the act of discarding the information about the specific position of the roulette wheel that effectively destroyed quantum superpositions.

A. The reduced state operator

To illustrate the concept of partial knowledge leading to classical behavior, we consider a universe made of a pair of two-state systems, each in a linear superposition of the states $|\uparrow\rangle$ and $|\downarrow\rangle$. In quantum mechanics we require such composite systems to remain separated in the sense that observables dealing only with the first subsystem, when applied to the

total system, should act only on the first subsystem.¹² Mathematically, the noncommutative operation we want is known as the tensor, cartesian, or direct product.⁸ This product pairs every possible state of the first system with every possible state of the second system. For example, the tensor product of two state vectors with matrix representations

$$|\theta\rangle = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix}, \quad |\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad (24)$$

is given by

$$|\theta\phi\rangle = |\theta\rangle|\phi\rangle = |\theta\rangle \otimes |\phi\rangle = \begin{pmatrix} \theta_1|\phi\rangle \\ \theta_2|\phi\rangle \end{pmatrix} = \begin{pmatrix} \theta_1\phi_1 \\ \theta_1\phi_2 \\ \theta_2\phi_1 \\ \theta_2\phi_2 \end{pmatrix}, \quad (25)$$

where the two shorthand notations used on the left are equivalent to the formal notation specified by \otimes (read *tensor*).⁸ A general state $|\psi\rangle$ for any two-state system is given by

$$|\psi\rangle = \sum_{ab} \psi_{ab}|ab\rangle = \psi_{11}|11\rangle + \psi_{12}|12\rangle + \psi_{21}|21\rangle + \psi_{22}|22\rangle, \quad (26)$$

which has the matrix representation

$$|\psi\rangle = \begin{pmatrix} \psi_{11} \\ \psi_{12} \\ \psi_{21} \\ \psi_{22} \end{pmatrix}. \quad (27)$$

The corresponding state operator is

$$\begin{aligned} \hat{\rho} &= |\psi\rangle\langle\psi| = \sum_{a_1b_1a_2b_2} \psi_{a_1b_1}\psi_{a_2b_2}^* |a_1b_1\rangle\langle a_2b_2| \\ &= \sum_{a_1b_1a_2b_2} \psi_{a_1b_1}\psi_{a_2b_2}^* |a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2| \end{aligned} \quad (28)$$

and has the (density) matrix representation

$$\hat{\rho} = \begin{pmatrix} \psi_{11}\psi_{11}^* & \psi_{11}\psi_{12}^* & \psi_{11}\psi_{21}^* & \psi_{11}\psi_{22}^* \\ \psi_{12}\psi_{11}^* & \psi_{12}\psi_{12}^* & \psi_{12}\psi_{21}^* & \psi_{12}\psi_{22}^* \\ \psi_{21}\psi_{11}^* & \psi_{21}\psi_{12}^* & \psi_{21}\psi_{21}^* & \psi_{21}\psi_{22}^* \\ \psi_{22}\psi_{11}^* & \psi_{22}\psi_{12}^* & \psi_{22}\psi_{21}^* & \psi_{22}\psi_{22}^* \end{pmatrix}. \quad (29)$$

The process of finding tensor products of general operators proceeds similarly. For example, if two operators have matrix representations

$$\hat{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}, \quad (30)$$

then their tensor product has the matrix representation

$$\begin{aligned} \hat{A} \otimes \hat{B} &= \begin{pmatrix} a_{11}\hat{B} & a_{12}\hat{B} \\ a_{21}\hat{B} & a_{22}\hat{B} \end{pmatrix} \\ &= \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}. \end{aligned} \quad (31)$$

Suppose that the composite operator, $\hat{O} = \hat{A} \otimes \hat{B}$, represents an observable of only the first subsystem A . That is, we want $\langle\hat{O}\rangle$ to not depend on the subsystem B . To do so we let $\hat{B} = \hat{I}_2$ be the two-dimensional identity operator so that

$$\hat{O} = \hat{A} \otimes \hat{I}_2 = \begin{pmatrix} a_{11} & 0 & a_{12} & 0 \\ 0 & a_{11} & 0 & a_{12} \\ a_{21} & 0 & a_{22} & 0 \\ 0 & a_{21} & 0 & a_{22} \end{pmatrix}. \quad (32)$$

Next, we combine Eqs. (32) and (29) to find the expectation value of \hat{O} via Eq. (16) in the state $|\psi\rangle$ to be

$$\begin{aligned} \langle\hat{O}\rangle_\psi &= \text{Tr}(\hat{\rho}\hat{O}) \\ &= (|\psi_{11}|^2 + |\psi_{12}|^2)a_{11} + (\psi_{21}\psi_{11}^* + \psi_{22}\psi_{12}^*)a_{12} \\ &\quad + (\psi_{11}\psi_{21}^* + \psi_{12}\psi_{22}^*)a_{21} + (|\psi_{21}|^2 + |\psi_{22}|^2)a_{22}. \end{aligned} \quad (33)$$

We now construct a way to discard information about subsystem B , leaving only information about subsystem A . We define a *reduced* or *local* state operator by performing a partial trace, that is, a trace over the B subsystem of Eq. (28). Namely,

$$\hat{\rho}_A = \text{Tr}_B(\hat{\rho}) = \sum_{a_1b_1a_2b_2} \psi_{a_1b_1}\psi_{a_2b_2}^* |a_1\rangle\langle a_2| \text{Tr}(|b_1\rangle\langle b_2|). \quad (34)$$

Because $\text{Tr}(|b_1\rangle\langle b_2|) = \text{Tr}(\langle b_2|b_1\rangle) = \langle b_2|b_1\rangle = \delta_{b_2b_1}$, the sum contracts to

$$\hat{\rho}_A = \sum_{a_1a_2} (\psi_{a_1}\psi_{a_2}^* + \psi_{a_2}\psi_{a_1}^*) |a_1\rangle\langle a_2|, \quad (35)$$

which has the (reduced density) matrix representation

$$\hat{\rho}_A = \begin{pmatrix} |\psi_{11}|^2 + |\psi_{12}|^2 & \psi_{11}\psi_{21}^* + \psi_{12}\psi_{22}^* \\ \psi_{21}\psi_{11}^* + \psi_{22}\psi_{12}^* & |\psi_{21}|^2 + |\psi_{22}|^2 \end{pmatrix} \quad (36)$$

or, equivalently,

$$\hat{\rho}_A = \begin{pmatrix} \text{Tr} \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} & \text{Tr} \begin{pmatrix} \rho_{13} & \rho_{14} \\ \rho_{23} & \rho_{24} \end{pmatrix} \\ \text{Tr} \begin{pmatrix} \rho_{31} & \rho_{32} \\ \rho_{41} & \rho_{42} \end{pmatrix} & \text{Tr} \begin{pmatrix} \rho_{33} & \rho_{34} \\ \rho_{43} & \rho_{44} \end{pmatrix} \end{pmatrix}. \quad (37)$$

We combine Eqs. (36) and (33) to show that

$$\text{Tr}(\hat{\rho}_A\hat{A}) = \langle\hat{O}\rangle_\psi = \text{Tr}(\hat{\rho}\hat{O}). \quad (38)$$

Thus, the reduced state operator $\hat{\rho}_A = \text{Tr}_B(\hat{\rho})$ is to subsystem A as the state operator $\hat{\rho}$ is to the composite system.

B. Bell state example

We now turn to a famous example of an entangled composite system, known as an EPR pair or Bell state,

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} +1 \\ 0 \\ 0 \\ -1 \end{pmatrix}. \quad (39)$$

This state is a superposition of both subsystems being $|\uparrow\rangle$ and both being $|\downarrow\rangle$, with equal probability.⁸ Physically, such a state occurs during the decay of positronium, where $|\uparrow\rangle$ and $|\downarrow\rangle$ correspond to the helicity of the resulting photons.¹⁶ This state is remarkable, particularly due to the perfect correlation of the two subsystems. If the first is found in $|\uparrow\rangle$, then the second will always be in $|\uparrow\rangle$, and *vice versa*.

From Eq. (29) the Bell state operator has the (density) matrix representation

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}, \quad (40)$$

which has nonzero nondiagonal terms and represents an entangled state. However, by Eq. (37), the reduced Bell state operator that characterizes the first subsystem has the matrix representation

$$\hat{\rho}_A = \text{Tr}_B(\hat{\rho}) = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (41)$$

which is diagonal and represents a mixed state.

The reduced state operator $\hat{\rho}_A$ has the same form as we found in Eq. (18), after the roulette wheel had stripped the quantum interference terms from the state operator. Hence, just as for the silver atom and the roulette wheel, the individual subsystems of the Bell state lack quantum properties, and instead are statistical states.⁸ Evidently, a manifestly quantum-mechanical system can be made of ostensibly classical pieces. Hence, the discarding of (quantum) information, wherein an entangled state is replaced by a mixed state, signals the emergence of classical behavior.

IV. CONTINUOUS DECOHERENCE AND QUANTUM BROWNIAN MOTION

Now that we have established the connection between the disappearance of the off-diagonal elements of the (density) matrix representation of the state operator with the emergence of classical behavior, we explore how such a process occurs in a continuous physical system. In addition to the state vector $|\psi\rangle$ and the state operator $\hat{\rho} = |\psi\rangle\langle\psi|$, we make use of the position representation of the state vector, the wave function $\psi(x) = \langle x|\psi\rangle$. In Sec. IV A we consider a free quantum mechanical system. In Sec. IV B we analyze the effect of a single collision between the system particle and environment particle. Finally, in Sec. IV C we place the system in thermal equilibrium with a statistical gas. This last system is reminiscent of classical Brownian motion and has served as a tractable example of a simple system interacting with a complex environment that is treated statistically.

A. The free system

According to the Schrödinger equation, the state vector $|\psi\rangle$ of a free particle of mass m evolves with time t according to

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \frac{\hat{p}^2}{2m} |\psi\rangle, \quad (42)$$

where \hat{p} is the momentum operator. Because $\hat{p} = \hat{p}^\dagger$ is Hermitian, the adjoint of Eq. (42) is

$$-i\hbar \frac{\partial}{\partial t} \langle\psi| = \langle\psi| \frac{\hat{p}^2}{2m}. \quad (43)$$

Together with Eq. (7), Eqs. (42) and (43) imply that the time derivative of the state operator is

$$\begin{aligned} \frac{\partial}{\partial t} \hat{\rho} &= \frac{\partial}{\partial t} |\psi\rangle\langle\psi| = \left(\frac{\partial}{\partial t} |\psi\rangle \right) \langle\psi| + |\psi\rangle \left(\frac{\partial}{\partial t} \langle\psi| \right) \\ &= \frac{\hat{p}^2}{i\hbar 2m} |\psi\rangle\langle\psi| - |\psi\rangle\langle\psi| \frac{\hat{p}^2}{i\hbar 2m}. \end{aligned} \quad (44)$$

We let $|x\rangle$ and $|y\rangle$ be eigenstates of definite position and multiply both sides of Eq. (44) by $\langle x|$ from the left and $|y\rangle$ from the right to find^{3,17}

$$\begin{aligned} \frac{\partial}{\partial t} \rho(x,y) &= \langle x| \frac{\partial}{\partial t} \hat{\rho} |y\rangle \\ &= \frac{1}{i\hbar 2m} (\langle x|\hat{p}^2|\psi\rangle\langle\psi|y\rangle - \langle x|\psi\rangle\langle\psi|\hat{p}^2|y\rangle) \end{aligned} \quad (45a)$$

$$\begin{aligned} &= \frac{1}{i\hbar 2m} \left[\left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right)^2 \langle x|\psi\rangle\langle\psi|y\rangle \right. \\ &\quad \left. - \left(\frac{\hbar}{i} \frac{\partial}{\partial y} \right)^2 \langle x|\psi\rangle\langle\psi|y\rangle \right] \end{aligned} \quad (45b)$$

$$= \frac{i\hbar}{2m} \left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right) \rho(x,y), \quad (45c)$$

where $\rho(x,y) = \langle x|\hat{\rho}|y\rangle = \langle x|\psi\rangle\langle\psi|y\rangle$ are the matrix elements of $\hat{\rho}$.^{8,18} These elements correspond to the probability amplitude to go from an initial state $|y\rangle$ to a final state $|x\rangle$ via an intermediate state $|\psi\rangle$.^{16,19} A laboratory system is always localized in space, so we expect $\rho(x,y) \rightarrow 0$ as $|x-y| \rightarrow \infty$. Note also that the energy eigenstate wavefunctions of the free particle (plane waves) have the form

$$\psi(x) = e^{i(px-Et)/\hbar} \quad (46)$$

and render Eq. (45) identically zero, as we would expect for stationary states.

B. Analyzing a single collision

We next investigate the one-dimensional collision of a single environment particle with a system (or Brownian) particle. We assume that the environment particle has mass m_e , precollision momentum p_e , and postcollision momentum \tilde{p}_e , and the system particle has mass m_s , precollision momentum p_s , and postcollision momentum \tilde{p}_s . For an ideal collision conservation of momentum and kinetic energy imply²⁰

$$\tilde{p}_s = \frac{m_s - m_e}{m_s + m_e} p_s + \frac{2m_s}{m_s + m_e} p_e, \quad (47a)$$

$$\tilde{p}_e = \frac{2m_e}{m_s + m_e} p_s - \frac{m_s - m_e}{m_s + m_e} p_e. \quad (47b)$$

We assume that the system particle is very massive compared to the environment particle, that is, $m_s \gg m_e$, and apply this approximation to Eq. (47) to obtain

$$\tilde{p}_s \approx p_s + 2p_e, \quad (48a)$$

$$\tilde{p}_e \approx 2\frac{m_e}{m_s} p_s - p_e. \quad (48b)$$

If we assume that the environment particle is moving much faster than the system particle, so $p_e/m_e \gg p_s/m_s$, then Eq. (48) becomes

$$\tilde{p}_s \approx p_s + 2p_e, \quad (49a)$$

$$\tilde{p}_e \approx -p_e. \quad (49b)$$

In quantum mechanics we can expand the two-particle pre- and postcollision position wavefunctions (or wave packets) in terms of plane wave momentum eigenstates. In analogy to the classical case, we assume that Eq. (49) holds for all momentum states. If x_s and x_e are the initial positions of the system and the environment particles, and $\varphi(p_e, p_s)$ is the momentum wave function, then immediately after the collision

$$\begin{aligned} \tilde{\psi}(x_e, x_s) &= \int \frac{d\tilde{p}_e d\tilde{p}_s}{2\pi\hbar} \varphi(\tilde{p}_e, \tilde{p}_s) e^{i(\tilde{p}_e x_e + \tilde{p}_s x_s)/\hbar} \\ &= \int |J| \frac{dp_e dp_s}{2\pi\hbar} \varphi(\tilde{p}_e, \tilde{p}_s) e^{i(\tilde{p}_e x_e + \tilde{p}_s x_s)/\hbar}, \end{aligned} \quad (50)$$

where the absolute value of the Jacobian determinant of the momentum transformation in Eq. (47) is $|J|=1$. We use the approximation (49) and define $\tilde{\varphi}(p_e, p_s) = \varphi(\tilde{p}_e, \tilde{p}_s)$, so that $\tilde{\psi}(x_e, x_s)$ becomes

$$\tilde{\psi}(x_e, x_s) \approx \int \frac{dp_e dp_s}{2\pi\hbar} \tilde{\varphi}(p_e, p_s) e^{i(p_e(2x_s - x_e) + p_s x_s)/\hbar} \quad (51a)$$

$$\approx \int \frac{dp_e dp_s}{2\pi\hbar} \tilde{\varphi}(p_e, p_s) e^{i(p_e \tilde{x}_e + p_s \tilde{x}_s)/\hbar}, \quad (51b)$$

where the changes in momenta due to the collision induce the new positions $\tilde{x}_s \approx x_s$ and $\tilde{x}_e \approx 2x_s - x_e$ in each of the momentum eigenstates.³

C. Treatment of a statistical environment

We place the quantum mechanical system in an environment containing an ideal gas, as shown in Fig. 3. To find the total state operator we use the composite system formalism we developed in Sec. III. The composite state operator $\hat{\rho}$ is

$$\hat{\rho} = \hat{\rho}_s \otimes \hat{\rho}_e, \quad (52)$$

where $\hat{\rho}_s$ is the state operator of the system and $\hat{\rho}_e$ is the state operator of the environment particle.^{8,12} We take x_s and y_s to be arbitrary system coordinates, and x_e and y_e to be the arbitrary environment particle coordinates, still in one dimension. We form matrix elements of Eq. (52) by multiplying both sides by $\langle x_s | \otimes \langle x_e |$ from the left and $|y_s\rangle \otimes |y_e\rangle$ from the right, so that

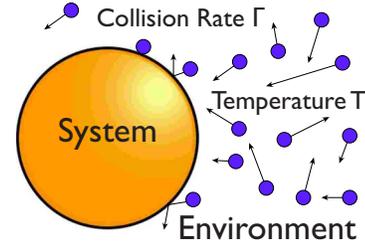


Fig. 3. (Color online) A cartoon of a quantum mechanical system undergoing collisions at a rate Γ with an ideal gas at temperature T . For simplicity, we consider the analogous one-dimensional system.

$$\langle \langle x_s | \otimes \langle x_e | \hat{\rho} | y_s \rangle \otimes | y_e \rangle \rangle = \langle x_s | \hat{\rho}_s | y_s \rangle \otimes \langle x_e | \hat{\rho}_e | y_e \rangle, \quad (53)$$

which can be written as

$$\rho(x_s, y_s, x_e, y_e) = \rho_s(x_s, y_s) \rho_e(x_e, y_e), \quad (54)$$

where the tensor product reduces to an ordinary product because the factors are scalars. If we assume that the collisions between system and environment particles are their only interactions, after a collision, we have

$$\tilde{\rho}(x_s, y_s, x_e, y_e) = \rho(\tilde{x}_s, \tilde{y}_s, \tilde{x}_e, \tilde{y}_e) = \rho_s(\tilde{x}_s, \tilde{y}_s) \rho_e(\tilde{x}_e, \tilde{y}_e). \quad (55)$$

As in Sec. III we now focus on the system, a subset of our universe. Following Eq. (34), we form the system's final reduced state operator by finding the partial trace over the environmental degrees of freedom of the total state operator,

$$\begin{aligned} \tilde{\rho}_s(x_s, y_s) &= \text{Tr}_e(\tilde{\rho}(x_s, y_s, x_e, y_e)) = \rho_s(\tilde{x}_s, \tilde{y}_s) \text{Tr}_e(\rho_e(\tilde{x}_e, \tilde{y}_e)) \\ &= \rho_s(x_s, y_s) \text{Tr}_e(\rho_e(2x_s - x_e, 2y_s - y_e)). \end{aligned} \quad (56)$$

Because the position basis is continuous, the trace is an integral rather than a sum.²¹ Working on the diagonal, we set $x_e = y_e$ and integrate to get³

$$\begin{aligned} \Lambda &\equiv \text{Tr}_e(\rho_e(2x_s - x_e, 2y_s - y_e)) \\ &= \int_{-\infty}^{\infty} dx_e \rho_e(2x_s - x_e, 2y_s - x_e) \end{aligned} \quad (57a)$$

$$= \int_{-\infty}^{\infty} d\xi \rho_e(\xi + 2(x_s - y_s), \xi). \quad (57b)$$

where $\xi = 2y_s - x_e$.

For a laboratory experiment localized in space the state operator and its derivatives are very small for large separations $|x_s - y_s|$. Thus, we expand the integrand of Λ in powers of $2(x_s - y_s)$ to second order to obtain

$$\begin{aligned} \Lambda &\approx \int_{-\infty}^{\infty} d\xi \rho_e(\xi, \xi) + 2(x_s - y_s) \int_{-\infty}^{\infty} d\xi \frac{\partial}{\partial X} \rho_e(X, \xi) \Big|_{X=\xi} \\ &\quad + 2(x_s - y_s)^2 \int_{-\infty}^{\infty} d\xi \frac{\partial^2}{\partial X^2} \rho_e(X, \xi) \Big|_{X=\xi}, \end{aligned} \quad (58)$$

where the derivatives act only on the first of the state operator's two arguments. In Sec. II we noted that the state operator has unit trace. Hence, the first term of Eq. (58) simplifies to

$$\int_{-\infty}^{\infty} d\xi \rho_e(\xi, \xi) = \text{Tr}(\hat{\rho}_e) = 1. \quad (59)$$

Now, we apply the definition of the momentum operator to the last two terms. We use Eq. (16) to identify the expectation value of the momentum operator,

$$\begin{aligned} \int_{-\infty}^{\infty} d\xi \frac{\partial}{\partial X} \rho_e(X, \xi) \Big|_{X=\xi} &= - \int_{-\infty}^{\infty} d\xi \frac{\hat{p}}{i\hbar} \rho_e(\xi, \xi) \quad (60a) \\ &= - \frac{1}{i\hbar} \text{Tr}(\hat{p} \hat{\rho}_e) = - \frac{1}{i\hbar} \langle \hat{p} \rangle = 0, \quad (60b) \end{aligned}$$

which vanishes because the environment particles are assumed to have random velocities.³ Similarly,

$$\int_{-\infty}^{\infty} d\xi \frac{\partial^2}{\partial X^2} \rho_e(X, \xi) \Big|_{X=\xi} = - \frac{1}{\hbar^2} \langle \hat{p}^2 \rangle. \quad (61)$$

Therefore, Eq. (58) becomes

$$\Lambda = 1 - \frac{2(x_s - y_s)^2}{\hbar^2} \langle \hat{p}^2 \rangle. \quad (62)$$

Because we assumed the environment to be an ideal one-dimensional gas, we know that

$$\frac{\langle \hat{p}^2 \rangle}{2m_e} = \frac{1}{2} kT, \quad (63)$$

or $\langle \hat{p}^2 \rangle = m_e kT$, where m_e is the mass of an environment particle, k is Boltzmann's constant, and T is the temperature of the environment.²² For a time interval Δt and a collision rate Γ the total change in the system state operator is

$$\Delta \rho_s = \Gamma \Delta t (\tilde{\rho}_s(x_s, y_s) - \rho_s(x_s, y_s)) \quad (64a)$$

$$= \Gamma \Delta t (\Lambda - 1) \rho_s(x_s, y_s). \quad (64b)$$

If we use Eqs. (62) and (63), Eq. (64) becomes

$$\Delta \rho_s = - 2\Gamma \Delta t (x_s - y_s)^2 \frac{m_e kT}{\hbar^2} \rho_s(x_s, y_s). \quad (65)$$

Thus, due to collisions only, the rate of change of the matrix elements of the system state operator is

$$\frac{\partial \rho_s}{\partial t} = - 2(x_s - y_s)^2 \frac{\Gamma m_e kT}{\hbar^2} \rho_s. \quad (66)$$

As we will illustrate by an example in Sec. V, Eq. (66) is a differential equation for exponential decay of the off-diagonal ($x_s \neq y_s$) elements.

Because the only forces on the system are due to environmental collisions, we may combine Eqs. (66) and (45) to obtain the total equation of motion for the system,

$$\frac{\partial}{\partial t} \rho_s = \frac{i\hbar}{2m_s} \left(\frac{\partial^2}{\partial x_s^2} - \frac{\partial^2}{\partial y_s^2} \right) \rho_s - 2(x_s - y_s)^2 \frac{\gamma m_s kT}{\hbar^2} \rho_s, \quad (67)$$

where we have made the conventional definition for the

dissipation $\gamma = \Gamma m_e / m_s$.³ Equation (67) is a special case of the master equation for quantum Brownian motion,^{5,6,9,23} and we now explore its significance.

V. DECOHERENCE OF A QUANTUM SIMPLE HARMONIC OSCILLATOR

We apply the general results of Eq. (67) to the example of a decohering quantum simple harmonic oscillator. As is well known,^{10,11} the wavefunction for the n th energy level of the one-dimensional harmonic oscillator of mass m and classical frequency ω is

$$\psi(x) = \frac{1}{\sqrt{n!}} \left[\sqrt{\frac{\hbar}{2m\omega}} \left(\frac{m\omega}{\hbar} x - \partial_x \right) \right]^n \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-m\omega x^2/2\hbar}. \quad (68)$$

The relation between the wavefunction and matrix elements of the system's state operator is

$$\rho_s(x, y) = \langle x | \psi \rangle \langle \psi | y \rangle = \psi(x) \psi^*(y), \quad (69)$$

so

$$\begin{aligned} \rho_s(x, y) &= \frac{1}{n!} \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} \left(\frac{\hbar}{2m\omega} \right)^n \left(\frac{m\omega}{\hbar} x - \partial_x \right)^n \\ &\quad \times \left(\frac{m\omega}{\hbar} y - \partial_y \right)^n e^{-m\omega x^2/2\hbar} e^{-m\omega y^2/2\hbar}. \quad (70) \end{aligned}$$

We next determine how this state operator varies with time when the oscillator is placed into thermal equilibrium with an ideal statistical gas. We notice that due to the macroscopically small \hbar^2 in its denominator, the last term of the master equation, Eq. (67), will dominate for all but microscopic separations $|x - y|$, and Eq. (67) simplifies to

$$\frac{\partial \rho_s}{\partial t} \approx - 2(x - y)^2 \frac{\gamma m kT}{\hbar^2} \rho_s, \quad (71)$$

with the solution

$$\rho_s(x, y, t) = \rho_s(x, y, 0) e^{-(2\gamma m kT/\hbar^2)(x - y)^2 t}. \quad (72)$$

It is conventional to introduce the separation-dependent decoherence time^{9,24}

$$t_d(x, y) = \frac{\hbar^2}{2\gamma m kT(x - y)^2}, \quad (73)$$

so that

$$\rho_s(x, y, t) = \rho_s(x, y, 0) e^{-t/t_d(x, y)}. \quad (74)$$

We see that the off-diagonal elements of the state operator's matrix representation vanish exponentially with time, and elements farther from the diagonal disappear faster than elements nearer to the diagonal. Because the quantum interference terms that define quantum superpositions exist in the off-diagonal elements, we see that the superposition states of the harmonic oscillator decay exponentially with time. To visualize this decay we plot in Fig. 4 the matrix elements of the state operator of a decohering simple harmonic oscillator initially in its third excited state.⁶ The light and dark regions correspond to peaks and valleys in a three-dimensional representation, which level out as time proceeds. In analogy

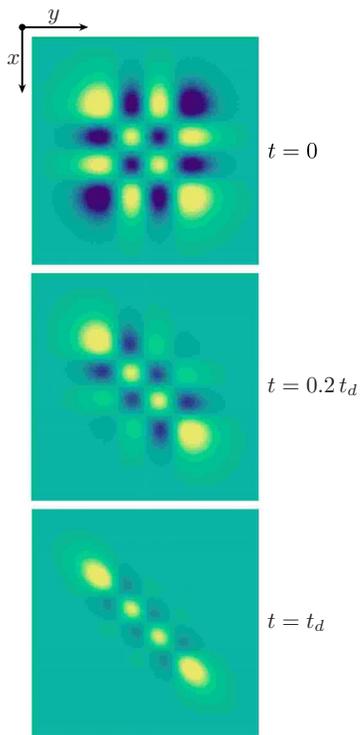


Fig. 4. (Color online) The matrix elements of the state operator $\rho_s(x, y, t)$ of a decohering quantum harmonic oscillator initially in its $n=3$ excited state, calculated using the approximate solution to the master equation given by Eq. (74). Dark shading indicates negative values, and light shading indicates positive values.

with Eqs. (18) and (41) the off-diagonal ($x \neq y$) elements decay, leaving a statistical, classical state down the diagonal of the state operator.

VI. CONCLUSION

We have offered three complementary arguments, each related to the origin of quantum-classical emergence using decoherence. In Sec. II we considered phase randomization through the coupling with a roulette wheel, establishing the connection between the off-diagonal elements of the state operator and quantum properties. In Sec. III we traced information out of a composite system, showing that subsystems could separately appear classical while together forming a quantum whole, and that such classical behavior is marked by a diagonal reduced state operator. In Sec. IV we considered the physical origins of such information leakage by way of a statistical environment. By tracing out the environment and focusing on the harmonic oscillator system in Sec. V, we were left with a diagonal, and hence classical, reduced state operator.

Although decoherence provides a physical way to explain the small pockets of classical behavior we observe, it does not attempt to answer the fundamental questions regarding the nature of measurement and interpretation.^{1,25} For instance, is our classical world just a reduction from the true universe, which ultimately exists as a single state operator over Hilbert space?⁹

Fortunately such questions are of greater philosophical than physical importance. However, the conventional interpretation of a measurement is not good enough for contem-

porary experiments in quantum mechanics.²⁶ Current efforts in quantum computation, for example, make use of decoherence theory to calculate the quality of a quantum state.¹ Although decoherence theory might not put the final nail in the coffin of Schrödinger's cat, its utility makes it a vital part of interpreting quantum mechanics.

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²³Equation (67) is missing the dissipation term, which damps the motion of the system. This damping is not that important in the regime in which we are looking. To develop a master equation with dissipation we would use Wigner's quasi-probability function in phase-space, improving the accuracy of our approximations (Ref. 29). Further background on the Wigner function is discussed in Refs. 27 and 28.

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