

# Decoherence challenges in Nanoscience: A Quantum Phase Space perspective

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## Abstract

Quantum decoherence, the process by which a quantum system loses its coherence through interaction with an environment and becomes classical-like, represents both the fundamental mechanism for the quantum-to-classical transition and a major challenge to realizing scalable nanoscale quantum technologies. This work introduces a novel theoretical framework based on Quantum Phase Space (QPS) to address the dual challenge of characterizing environment-selected pointer states and modeling decoherence dynamics across different regimes. Within this framework, pointer states for particle motion are identified as the minimum-uncertainty states, those that saturate the quantum uncertainty relation, thereby constituting the closest quantum analogue to classical phase-space points. The structure of the QPS, encoded in a variance-covariance matrix, is shown to be directly shaped by environmental properties. A time-independent matrix corresponds to Markovian (memoryless) decoherence, described by constant diffusion and friction coefficients, while a time-dependent matrix captures non-Markovian dynamics, characterized by environmental memory and information backflow. This unified geometric formalism, applied to both Lindblad and Non-Markovian master equations, enables us to derive explicit relations between environmental parameters and phase-space structure, as demonstrated in a specific illustrative example. This approach has the potential to serve as a powerful tool for modeling decoherence in nanoscience and could inform new principles for designing mitigation strategies and harnessing non-Markovian effects for quantum technologies. The QPS framework may thus bridge fundamental theory and practical quantum engineering, offering a promising coherent pathway to understand, control, and exploit decoherence at the nanoscience frontier.

**Keywords:** Quantum decoherence, Pointer states, Nanoscience, Quantum technologies, Quantum phase space

# 1 Introduction

Quantum decoherence stands as one of the most profound phenomena in modern physics, representing the loss of quantum coherence due to the interaction between a quantum system and its surrounding environment. This process not only lies at the heart of fundamental questions concerning the quantum-to-classical transition and the measurement problem [1, 2, 3, 4, 5, 6], but also poses significant challenges in nanoscience and nanotechnology, particularly for the realization of scalable quantum technologies [7, 8]. At the nanoscale, where quantum effects become prominent and environmental interactions are inevitable, decoherence emerges as the dominant mechanism that governs the stability, performance, and ultimate feasibility of quantum devices such as quantum computers, sensors, and metrological systems [9].

Unlike classical physics, quantum mechanics permits systems to exist in coherent superposition states [1, 2, 10]. Yet, the macroscopic world appears definite and classical-like. Quantum decoherence provides the explanatory bridge between these two regimes: through continuous environmental monitoring, the system's state evolves into a preferred basis of so-called pointer states. These pointer states are the system state that remain robust through environmental entanglement, thus emulating classical behavior [2, 11]. However, despite its conceptual clarity, a complete and mathematically rigorous description of decoherence, particularly the identification and dynamical evolution of pointer states in realistic nanoscale environments, remains an open theoretical challenge [12, 13, 14, 15, 16]. Nanoscience, the discipline concerned with materials and devices at the nanometer scale, serves as both the primary arena for observing decoherence and the technological frontier where its control is most urgently needed [17, 18]. In nanodevices, ranging from quantum dots [19], nanomechanical resonators [17], and molecular assemblies to superconducting qubits, decoherence dictates whether particle motion exhibits quantum coherence or classical trajectories. The distinction between Markovian (memoryless) and non-Markovian (memory-retaining) decoherence processes adds further complexity, affecting modeling strategies, control protocols, and the design of fault-tolerant quantum systems [8, 16, 20].

In this work, we address these challenges by introducing a novel theoretical framework rooted in the concept of Quantum Phase Space (QPS). This approach provides a unified and mathematically rigorous description of pointer states as minimum-uncertainty states that saturate the quantum uncertainty relation, thereby offering a natural connection between quantum dynamics and classical phase-space trajectories [2, 21, 22, 23]. We also show how the QPS formalism can systematically account for both Markovian and non-Markovian environments, enabling a more accurate modeling of decoherence dynamics. The paper is structured as follows. In Section 2, we review the foundational principles of quantum decoherence and the role of pointer states in multi-level quantum systems. Section 3 examines the implications of decoherence for particle motion in nanoscience and quantum technologies, emphasizing the distinction between Markovian and non-Markovian regimes. Section 4 introduces the quantum phase space framework and establishes its relation to pointer state selection. Section 5 provides an illustrative example to demonstrate, through both Markovian and non-Markovian master equations, how environmental properties shape the structure of quantum phase space and the decoherence process. Finally, we conclude with a discussion of the broader implications of our approach for quantum technology and fundamental physics. The following notational conventions are used: quantum operators are represented by boldface symbols, and non-operator quantities, including eigenvalues, are set in regular font.

## 2 Quantum decoherence and pointer states

Pointer states are the quantum states that remain stable when the system interacts with its environment. They are the states that decoherence does not "destroy" [2, 24]. Decoherence tends to destroy superpositions through environmental entanglement, but pointer states are the ones that do not become entangled in a way that destroys their classical-like behavior. They are the states that survive environmental monitoring. We can think of them as the eigenstates of the system observables that are continuously 'measured' by the environment [1, 3]. A first way to technically define pointer states is then to consider them as the eigenstates (or approximate eigenstates) of the system operators that the environment continuously monitors. Because the environment acts like a measuring device, it selects a preferred basis in which superpositions rapidly

decay. This basis is formed by the set of pointer states and is then called the pointer basis[5, 25]. Suppose the interaction Hamiltonian is :

$$H_{int} = \sum_k \mathbf{A}_k \otimes \mathbf{B}_k \quad (1)$$

where operators  $\mathbf{A}_k$  acts on the system and  $\mathbf{B}_k$  on the environment. Pointer states  $|\alpha_i\rangle$  satisfy :

$$\mathbf{A}_k |\alpha_i\rangle \approx a_{ik} |\alpha_i\rangle \quad (2)$$

The relation (2) means that pointer states are considered as approximate eigenstates of the operators  $\mathbf{A}_k$  that couple to the environment:

- For an environment that measures momentum, the pointer states are momentum eigenstates.
- If the environment measures position then pointer states are localized position states.
- If it measures energy, pointer states are energy eigenstates.
- If it measures a spin axis, pointer states are spin states along that axis, etc.

The evolution of the density operator offers another viewpoint for defining and visualizing both the emergence of pointer states and the decoherence phenomenon. Consider the system starting in a pure state  $|\psi_S\rangle$  and the environment in an initial state  $|e_0\rangle$ . Suppose the interaction between the system and environment begins at this initial time ( $t = 0$ ). For  $t > 0$ , entanglement arises between the state of the system and that of the environment. The entangled global state  $|\psi_{SE}\rangle$  can be written in the following form:

$$|\psi_{SE}\rangle = \sum_{i=1}^n C^i (|s_i\rangle \otimes |e_i\rangle) \quad (3)$$

where  $\{|s_i\rangle\}$  is a basis in the system state space and  $\{|e_i\rangle\}$  the basis of the environment state space correlated with  $\{|s_i\rangle\}$ . The canonical density operator which describes the system-environment entanglement is then :

$$\rho_{SE} = |\Psi_{SE}\rangle \langle \Psi_{SE}| = \sum_{i=1}^n \sum_{j=1}^n C^i C^{*j} (|s_i\rangle \langle s_j| \otimes |e_i\rangle \langle e_j|) \quad (4)$$

the density operator  $\rho_S = \rho$  of the system can be obtained by taking the partial trace over the environment degree of freedom :  $\rho = Tr_E(\rho_{SE})$ . Explicitly:

$$\rho = \sum_{k=1}^n \langle e_k | \rho_{SE} | e_k \rangle = \sum_{k=1}^n \sum_{i=1}^n \sum_{j=1}^n C^i C^{*j} (|s_i\rangle \langle s_j| \langle e_k | e_i \rangle \langle e_j | e_k \rangle) = \sum_{i=1}^n \sum_{j=1}^n \rho_j^i (|s_i\rangle \langle s_j|) \quad (5)$$

with

$$\rho_j^i = \sum_{k=1}^n C^i C^{*j} (\langle e_k | e_i \rangle \langle e_j | e_k \rangle) \quad (6)$$

$\{|s_i\rangle\}$  is the pointer basis of the system if, for the environment basis  $\{|e_i\rangle\}$  correlated with it, we have the following relation:

$$\langle e_i(t) | e_j(t) \rangle \simeq \delta_j^i = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \quad \text{for } t \gg \tau_D \quad (7)$$

in which  $\tau_D$  is called the decoherence time: it is the characteristic time scale after which decoherence effects become significant. We have then

$$\rho_j^i(t) \simeq \sum_{k=1}^n C^i C^{*j} \delta_i^k \delta_k^j = \begin{cases} |C^i|^2 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \quad \text{for } t \gg \tau_D \quad (8)$$

which is equivalent to writing for the system's density operator :

$$\rho(t) \simeq \sum_{i=1}^n \rho_i^i |s_i\rangle\langle s_i| = \sum_{i=1}^n |C^i|^2 |s_i\rangle\langle s_i| \quad \text{for } t \gg \tau_D \quad (9)$$

Relations (7), (8), and (9) are equivalent and describe the phenomenon of decoherence, which consists of a rapid decay of the off-diagonal terms of the density matrix for  $t > \tau_D$ . Indeed, these terms represent the existence of coherent superpositions among pointer states. For  $t \gg \tau_D$ , the matrix representation of the density operator in the pointer basis becomes approximately diagonal. The density operator then becomes an incoherent combination (statistical mixture) of pointer states: the diagonal elements  $\rho_i^i = |C_i|^2$  simply represent classical-like probabilities of finding the system in a defined pointer state.

### 3 Particle motion decoherence in Nanoscience and quantum technologies

Quantum decoherence in particle motion refers to the loss of quantum coherence in the spatial or motional degrees of freedom of a particle due to environmental interactions [1, 2, 26]. At the nanoscale (approximately between  $1nm = 10^{-9}m$  and  $100nm = 10^{-7}m$ ), this process fundamentally determines whether particle motion exhibits quantum behavior (superposition, interference) or classical trajectories. The distinction between Markovian (memoryless environment) and non-Markovian (memory-retaining environment) decoherence processes is critical for accurately modeling, controlling, and harnessing quantum motion in nanodevices [4, 8, 27, 28].

**3.1 Markovian and non-Markovian regimes in nanoscale particle motion decoherence**  
In nanoscience, particle motion, whether of negatons, excitons, nanoparticles, or nanomechanical resonators, is governed by quantum mechanics but is highly susceptible to decoherence [29]. The spatial superposition of a particle's wavefunction decays due to coupling with environmental degrees of freedom (phonons, photons, charge fluctuators, defect, impurities, etc) [26]. The timescale and nature of this decay depend critically on whether the environment is Markovian or non-Markovian [30]. Understanding these regimes guides material choice and device design, e.g., using purified silicon to reduce non-Markovian nuclear spin noise in spin qubits [9, 27].

**Markovian decoherence in particle motion:** under conditions of weak coupling, high temperature, and a broadband environment (e.g., negaton-phonon scattering in mesoscopic conductors), decoherence is approximately memoryless i.e. Markovian. The off-diagonal elements of the reduced density matrix for a particle in a spatial superposition of separation  $\Delta x = |x - x'|$  decay exponentially:

$$\rho(x, x', t) = \langle x | \rho(t) | x' \rangle = \rho(x, x', 0) \exp \left[ -\Gamma t (\Delta x)^2 \right] \quad (10)$$

where  $\Gamma = \frac{2m\gamma k_B T}{\hbar^2}$  is the constant decoherence rate,  $m$  is the particle mass,  $\gamma$  is the friction coefficient, and  $T$  is the temperature. This Markovian description applies, for instance to :

- Negaton transport in quantum dots at  $T > 1$  K, where negaton-negaton scattering provides rapid environmental relaxation.
- Nanomechanical resonators in low-pressure gas environments ( $P \sim 1\text{--}100$  Pa), where frequent gas collisions create memoryless damping [17].

**Non-Markovian decoherence in particle motion:** in contrast, when the environment has structure, long correlation times, or strong coupling, decoherence becomes non-Markovian. The expression for the off-diagonal elements of the density matrix is then

$$\rho(x, x', t) = \rho(x, x', 0) \exp \left[ -\Gamma(t) (\Delta x)^2 \right] \quad (11)$$

In contrast to equation (10), the parameter  $\Gamma(t)$  in equation (11) is time-dependent and can even decrease temporarily (recoherence), indicating quantum information backflow from environment to system (reactive environment). Examples of non-Markovian processes in Nanoscience include:

- Quantum dots in photonic bandgap materials, where suppressed density of states leads to photon localization and reversible decoherence.
- Nanomechanical resonators coupled to two-level systems (defects) at millikelvin temperatures, where coherent energy exchange creates non-exponential ring-down [18].

### 3.2 Quantum technologies and motional qubits

Quantum technologies exploit coherent particle motion for information processing, sensing, and communication (motional qubits). The coherence time of motional qubits, whether charge, phononic, or mechanical, is ultimately limited by decoherence, whose Markovian or non-Markovian character dictates control strategies. Markovian regimes permit simple exponential models and conventional dynamical decoupling. Non-Markovian regimes require advanced techniques: reservoir engineering, tailored pulse sequences that synchronize with backflow, and error correction adapted to non-exponential decay [15, 27, 31, 32].

**Charge qubits in quantum dots:** the motion of a negaton between two quantum dots constitutes a charge qubit. Its decoherence is dominated by charge noise and phonon coupling. In typical semiconductor environments, this is often treated as Markovian at elevated temperatures, yielding exponential dephasing ( $\tau_D \simeq T_2^* \sim 1\text{ns} = 10^{-9}\text{s}$ ) [19]. However, at low temperatures ( $T < 100 \text{ mK}$ ), the noise spectrum becomes structured, revealing non-Markovian signatures that must be accounted for in high-fidelity control[30].

**Nanomechanical qubits:** a nanomechanical resonator's center-of-mass motion can, in principle, be prepared in a spatial superposition. Decoherence arises from coupling to thermal phonons, radiation, and defects. In the Markovian regime (e.g., moderate vacuum,  $T > 100 \text{ mK}$ ), energy decay is exponential and described by a constant quality factor  $Q$ . In the non-Markovian regime (cryogenic, high-strain conditions), interaction with two-level systems leads to complex decay profiles and memory effects, impacting sensing performance and quantum state lifetime [18, 29].

### 3.3 Challenges related to decoherence in particle motion

Understanding and controlling decoherence is pivotal for exploiting the quantum properties of nanoscale particle motion. The journey from fundamental characterization to practical mitigation involves navigating a series of interconnected challenges, particularly when environments exhibit memory (non-Markovian dynamics). These challenges span experiment, engineering and theory defining the current frontier of the field:

- **Characterizing decoherence regimes:** Determining whether particle motion in a given nanoscale device undergoes Markovian or non-Markovian decoherence is nontrivial. This requires measuring temporal decay profiles, spectral densities, and correlation functions of environmental noise [16, 27].
- **Modeling and simulation:** Non-Markovian dynamics are computationally demanding to simulate. Developing efficient numerical methods is essential for accurate device prediction [20, 33].
- **Mitigation in non-Markovian environments:** While Markovian decoherence can often be mitigated with standard error correction, non-Markovian decoherence requires environment-aware strategies[34]: engineering bandgaps to suppress emission, using defect-free materials, or exploiting memory effects for enhanced sensing.
- **Harnessing non-Markovianity:** A paradigm shift is emerging: rather than suppressing all decoherence, non-Markovian memory effects can be harnessed for quantum advantage [20, 30, 35, 36].
- **Scalability with motional qubits:** As quantum devices scale, cross-talk between motional degrees of freedom and collective decoherence channels become significant. Managing these in both Markovian and non-Markovian contexts is critical for multi-qubit processors and sensor arrays [37, 38].

- **Mathematical-Physical framework for pointer states description:** A significant theoretical and practical challenge is the identification of pointer states. In particle motion, these correspond to localized positions or well-defined motional states that are least affected by the environment[14, 2]. A unified mathematical-physical framework that can systematically describe pointer states for both Markovian and non-Markovian environments would fundamentally transform decoherence management. The development of such a framework would directly address the challenges of characterization, mitigation, and scalability by providing a first-principles roadmap for coherence preservation in nanoscale particle motion. In the next sections, we will show how an approach grounded in quantum phase space theory may offer a promising path to fulfilling this requirement. This approach inherently unifies the description of decoherence regimes by casting the complementary dynamics of coherence decay and pointer state selection into a single geometric representation.

## 4 Quantum phase space perspective on decoherence

### 4.1 Identification of pointer states for particle motion

According to decoherence theory, when the motion of a particle is subjected to the effect of the environment, there will be through this interaction a selection of pointer states  $|\alpha\rangle$ , which form the pointer basis  $\{|\alpha\rangle\}$  so that the state of motion can be described with a density operator  $\rho$  given by the following relation (decomposition in the pointer basis):

$$\rho(t) = \iint \rho(\alpha, \beta, t) |\alpha\rangle\langle\beta| d\alpha d\beta \Leftrightarrow \rho(\alpha, \beta, t) = \langle\alpha|\rho(t)|\beta\rangle \quad (\text{continuous basis}) \quad (12)$$

The existence of decoherence phenomenon means that we have the following relation :

$$\rho(\alpha, \beta, t) \simeq 0 \quad \text{if } \alpha \neq \beta \quad \text{for } t \gg \tau_D \quad (13)$$

in which the parameter  $\tau_D$  is the decoherence time .

An explicit description of decoherence hinges on a key unknown: the set of pointer states  $|\alpha\rangle$  that are selected by the environment. Physically, these should correspond to the most stable, quasi-classical descriptions of the particle's trajectory. Consequently, the search naturally focuses on the momentum eigenstates  $|p\rangle$ , the position eigenstates  $|x\rangle$  (like in the relations (10) and (11)), or hybrid states (like coherent states) that blend both properties. Indeed, it is the position and momentum operators that are often involved in the expression of the interaction Hamiltonian. In other words, the environment's action constitutes a form of continuous measurement of these quantities through position-sensitive potentials and momentum-sensitive scattering processes for instance [1, 3]. Crucially, any rigorous selection or identification of pointer states must incorporate the constraints of the uncertainty principle. A rigorous framework for selecting pointer states must explicitly respect the quantum uncertainty relation, which is

$$\sigma_{xx}\sigma_{pp} - (\sigma_{px})^2 \geq \frac{(\hbar)^2}{4} \quad (14)$$

where  $\sigma_{pp}, \sigma_{xx}$  and  $\sigma_{px}$  are respectively variances and covariance of momentum and coordinate:

- Selecting a pure momentum eigenstate  $|p\rangle$  implies  $\sigma_{pp} = 0$ , which is unphysical as it requires  $\sigma_{xx} = \infty$
- Selecting a pure position eigenstate  $|x\rangle$  implies  $\sigma_{xx} = 0$ , which is equally unphysical as it requires  $\sigma_{pp} = \infty$ . If we rigorously take this conclusion into account, it is clear that even relations (10) and (11) are ill-defined

Therefore, viable pointer states must be minimum-uncertainty states that optimally localize both position and momentum within the bounds of the uncertainty principle. Furthermore, in classical physics, the one-dimensional motion of a particle is fully described by its instantaneous position  $x(t)$  and momentum  $p(t)$ . The set of all possible simultaneous pairs  $(p, x)$  defines the particle's classical phase space, and each such pair represents an elementary basis state of motion. It follows that the quantum pointer states  $|\alpha\rangle$  should be those that most closely approximate these classical basis states  $(p, x)$ . According to the uncertainty relation (14), the existence of state with exact simultaneous determination of  $p$  and  $x$  is impossible in quantum

physics ( $\sigma_{xx} = 0$  and  $\sigma_{pp} = 0$ ). The quantum states that most closely resemble the classical phase-space point  $(p, x)$  are not eigenstates of position or momentum alone, but rather the states denoted  $|\langle z \rangle\rangle$ , which saturate the uncertainty relation [1, 21, 39]. These minimum-uncertainty states, called joint momentum-coordinate states form the cornerstone for defining a quantum phase space, as they provide the closest possible quantum analogue to a classical point  $(p, x)$ . [1, 2, 21, 22, 23, 40]. The coordinate wavefunction corresponding to these states are given by the following relation [21]:

$$\langle x | \langle z \rangle \rangle = \frac{1}{(2\pi\chi)^{1/4}} e^{-\frac{\mathcal{B}}{\hbar^2}(x - \langle x \rangle)^2 + \frac{i}{\hbar}\langle p \rangle x} \quad (15)$$

in which :

- $\langle p \rangle$  and  $\langle x \rangle$  are respectively the expectation values of momentum and coordinate operators,  $\mathbf{p}$  and  $\mathbf{x}$  corresponding to a state  $|\langle z \rangle\rangle$  itself

$$\langle x \rangle = \langle \langle z \rangle | \mathbf{x} | \langle z \rangle \rangle \quad \text{and} \quad \langle p \rangle = \langle \langle z \rangle | \mathbf{p} | \langle z \rangle \rangle \quad (16)$$

- $\mathcal{B}$  is a parameter which is related to the variance and covariance,  $\sigma_{pp} = \mathcal{P}, \sigma_{xx} = \chi$  and  $\sigma_{px} = \mathcal{Q}$  of momentum and coordinate operators,  $\mathbf{p}$  and  $\mathbf{x}$  corresponding to the states  $|\langle z \rangle\rangle$

$$\mathcal{B} = \frac{\hbar^2}{4\chi} \left(1 - \frac{2i}{\hbar}\mathcal{Q}\right) = \frac{\mathcal{P}}{1 + \frac{4\mathcal{Q}^2}{\hbar^2}} \left(1 - \frac{2i}{\hbar}\mathcal{Q}\right) \quad (17)$$

$$\begin{cases} \mathcal{P} = \langle \langle z \rangle | (\mathbf{p} - \langle p \rangle)^2 | \langle z \rangle \rangle = \langle \langle z \rangle | (\mathbf{p})^2 | \langle z \rangle \rangle - (\langle p \rangle)^2 \\ \chi = \langle \langle z \rangle | (\mathbf{x} - \langle x \rangle)^2 | \langle z \rangle \rangle = \langle \langle z \rangle | (\mathbf{x})^2 | \langle z \rangle \rangle - (\langle x \rangle)^2 \\ \mathcal{Q} = \frac{1}{2} \langle \langle z \rangle | (\mathbf{p} - \langle p \rangle)(\mathbf{x} - \langle x \rangle) + (\mathbf{x} - \langle x \rangle)(\mathbf{p} - \langle p \rangle) | \langle z \rangle \rangle = \frac{1}{2} \langle \langle z \rangle | \mathbf{p}\mathbf{x} + \mathbf{x}\mathbf{p} | \langle z \rangle \rangle - \langle p \rangle \langle x \rangle \end{cases} \quad (18)$$

$\mathcal{P}, \chi$  and  $\mathcal{Q}$  correspond to the saturation of the uncertainty relation (14),

$$\det[\mathcal{G}] = \mathcal{P}\chi - (\mathcal{Q})^2 = \frac{(\hbar)^2}{4} \quad \text{where} \quad \mathcal{G} = \begin{pmatrix} \mathcal{P} & \mathcal{Q} \\ \mathcal{Q} & \chi \end{pmatrix} \quad (19)$$

$\mathcal{G}$  is the momentum-coordinate variances-covariance matrix corresponding to the state  $|\langle z \rangle\rangle$ .

It can be shown that the states  $|\langle z \rangle\rangle$  are eigenstates of the operator  $\mathbf{z} = \mathbf{p} - \frac{2i}{\hbar}\mathcal{B}\mathbf{x}$ . The corresponding eigenvalue equation is

$$\mathbf{z}|\langle z \rangle\rangle = \left[ \langle p \rangle - \frac{2i}{\hbar}\mathcal{B}\langle x \rangle \right] |\langle z \rangle\rangle = \langle z \rangle |\langle z \rangle\rangle \quad (20)$$

this eigenvalue equation justifies the notation  $|\langle z \rangle\rangle$ .

The Quantum Phase Space (QPS) is defined as the set  $\{(\langle p \rangle, \langle x \rangle)\}$  of the possible values of the expectation values pair  $(\langle p \rangle, \langle x \rangle)$  for given values of the variances and covariance  $\mathcal{P}, \chi$  and  $\mathcal{Q}$ .

The identification of the pointer states  $|\alpha\rangle = |\langle z \rangle\rangle$ , permits to have the following decomposition of the density operator  $\rho$ , for any arbitrary state, in the pointer basis  $\{|\langle z \rangle\rangle\}$ :

$$\rho(t) = \iiint \rho(\langle z \rangle, \langle z' \rangle, t) |\langle z \rangle\rangle \langle \langle z | \frac{d\langle p \rangle d\langle x \rangle}{h} \frac{d\langle p' \rangle d\langle x' \rangle}{h} \iff \rho(\langle z \rangle, \langle z' \rangle, t) = \langle \langle z \rangle | \rho(t) | \langle z' \rangle \rangle \quad (21)$$

According to these results, the concept of QPS permits the exact identification of the pointer state  $|\alpha\rangle = |\langle z \rangle\rangle$ . This identification provide a new mathematical framework for the study of decoherence.

## 4.2 Relations between environment properties, decoherence regime and the structure of the QPS

Based on the results of the previous section, there is a correspondence between the set of pointer states for a particle's motion and its QPS. Consequently, the characteristics of the environment, which are reflected in the nature of the pointer states, are directly linked to the structure of the particle's quantum phase space. This structure is defined by the variances-covariance matrix . It follows that the properties of the environment are also described by these quantities. Two main cases can be distinguished : stationary environment and reactive environment.

**Stationary environment:** This case occurs when the environment's intrinsic characteristics, such as its spectral density, temperature, and correlation functions, are not significantly perturbed or reconfigured by its interaction with the particle. Conceptually, the environment is assumed to be so large or have such fast internal dynamics that the energy and information exchanged with the particle cause negligible back-action. While the environment inevitably captures information about the particle's state (for example, through scattering or field emissions), this transfer does not substantially alter the environment's global statistical properties or its future dynamical rules. Consequently, the environment retains no lasting "memory" of any specific interaction event; it resets rapidly to its equilibrium state, behaving as a memoryless Markovian reservoir.

As will be illustrated in the detailed example studied later, this type of environment corresponds precisely to the Markovian limit of decoherence. In this regime, the system's dynamics are local in time, described by master equations with constant damping rates, such as the Lindblad form. This theoretical description is physically justified when the environment's correlation time is vanishingly short compared to the system's dynamical timescale. The mathematical signature of this limit within our quantum phase-space framework is that the corresponding variance-covariance matrix for the environmental noise is time-independent, reflecting stationary statistical properties. It is this constancy in the second-order moments that formally justifies the designation "stationary" for the environment in this model. This stationarity ensures that the decoherence channels and diffusion processes they induce are uniform over time, leading to predictable, exponential decay of coherences.

$$\dot{\mathcal{X}} = \frac{d\mathcal{X}}{dt} = 0 \quad \dot{\mathcal{P}} = \frac{d\mathcal{P}}{dt} = 0 \quad \dot{\mathcal{Q}} = \frac{d\mathcal{Q}}{dt} = 0 \quad \dot{\mathcal{G}} = \frac{d\mathcal{G}}{dt} = \begin{pmatrix} \dot{\mathcal{P}} & \dot{\mathcal{Q}} \\ \dot{\mathcal{Q}} & \dot{\mathcal{X}} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \quad (22)$$

**Reactive environment (Non-Markovian):** This regime describes an environment whose intrinsic physical and statistical properties, such as its effective spectral density, temperature distribution, and, most crucially, its temporal correlation functions, are notably perturbed and reshaped by the particle's presence and dynamics. Unlike a passive, Markovian bath that remains inert and unchanging, a reactive environment dynamically adapts to the ongoing interaction. It does not simply act as a sink for information; rather, the absorption of information about the particle's state (e.g., its position, momentum, or internal energy) induces a structural or dynamical change within the environment itself. This exchange creates a bidirectional feedback loop: the system influences the environment, and the environment's modified state, in turn, exerts a new influence back on the system at a later time. This is the essence of a memory effect; the environment effectively retains a non-trivial, dynamical trace of past interactions, which actively influences the future evolution of the system's quantum coherences.

Consequently, the decoherence process becomes history-dependent. The rate and pathways of quantum information loss are no longer determined solely by the system's instantaneous state but are contingent upon the entire past sequence of system-environment interactions. This case, to be illustrated with a concrete example subsequently, epitomizes the non-Markovian regime of decoherence, moving beyond the standard Lindblad/master equation framework. Mathematically, this complex, temporally non-local behavior is captured by a time-dependent variance-covariance matrix for the environmental noise. This temporal dependence signifies that the statistical moments (the "noise strength" and inter-mode correlations) governing the environmental fluctuations are not stationary but evolve in response to the system's prior history, providing a direct quantitative signature of the environment's reactive and memory-bearing nature.

$$\dot{\mathcal{X}} = \frac{d\mathcal{X}}{dt} \neq 0 \quad \dot{\mathcal{P}} = \frac{d\mathcal{P}}{dt} \neq 0 \quad \dot{\mathcal{Q}} = \frac{d\mathcal{Q}}{dt} \neq 0 \quad \dot{\mathcal{G}} = \frac{d\mathcal{G}}{dt} = \begin{pmatrix} \dot{\mathcal{P}} & \dot{\mathcal{Q}} \\ \dot{\mathcal{Q}} & \dot{\mathcal{X}} \end{pmatrix} \neq 0 \quad (23)$$

## 5 Example study with Master equations

To illustrate the relationship between environmental properties, the decoherence regime, and the structure of the particle's quantum phase space, we consider in this section the evolution of a state analogous to pointer states. This state shares the same variance-covariance matrix as a true pointer state but possesses time-dependent expectation values for position and momentum, reflecting the existence of particle motion.

The corresponding density operator is:

$$\rho(t) = |\langle z_0(t) \rangle \rangle \langle \langle z_0(t) \rangle| = \iiint \rho(\langle z \rangle, \langle z' \rangle, t) | \langle z \rangle \rangle \langle \langle z \rangle| \frac{d\langle p \rangle d\langle x \rangle}{h} \frac{d\langle p' \rangle d\langle x' \rangle}{h} \quad (24)$$

with

$$\rho(\langle z \rangle, \langle z' \rangle, t) = \langle \langle z \rangle | \rho(t) | \langle z \rangle \rangle = \langle \langle z \rangle | \langle z_0(t) \rangle \rangle \langle \langle z_0(t) \rangle | \langle z \rangle \rangle \quad (25)$$

From equation (25), together with relations (15), (17), and (19), one can deduce the explicit expression of  $\rho(\langle z \rangle, \langle z' \rangle, t)$ :

$$\rho(\langle z \rangle, \langle z' \rangle, t) = e^{-\frac{1}{8}[(\langle y_0 \rangle) \mathcal{G}^{-1}(\langle y_0 \rangle)^T + (\langle y'_0 \rangle) \mathcal{G}^{-1}(\langle y'_0 \rangle)^T] + \frac{i}{2\hbar}[(\langle x_0 \rangle + \langle x' \rangle)(\langle p_0 \rangle - \langle p' \rangle) - (\langle x_0 \rangle + \langle x' \rangle)(\langle p_0 \rangle + \langle p' \rangle)]} \quad (26)$$

with

$$\begin{aligned} \langle y_0 \rangle &= (\langle p_0 \rangle - \langle p \rangle) & \langle x_0 \rangle + \langle x' \rangle) & \mathcal{G}^{-1} = \frac{1}{\det[\mathcal{G}]} \begin{pmatrix} \mathcal{X} & -\mathcal{Q} \\ -\mathcal{Q} & \mathcal{P} \end{pmatrix} = \frac{4}{\hbar^2} \begin{pmatrix} \mathcal{X} & -\mathcal{Q} \\ -\mathcal{Q} & \mathcal{P} \end{pmatrix} \\ \langle y'_0 \rangle &= (\langle p_0 \rangle - \langle p' \rangle) & \langle x_0 \rangle + \langle x' \rangle) \end{aligned}$$

On one hand, equation (26) allows for the direct calculation of the time derivative of  $\rho(\langle z \rangle, \langle z' \rangle, t)$ . On the other hand, this calculation can also be performed using standard master equations, such as the Lindblad equation for the Markovian case or time-convolutionless (TCL)-type equations for the non-Markovian case. The identification of the results from these two approaches enables the determination of explicit relationships between the coefficients characterizing the environment in these master equations and the variance-covariance matrix, which corresponds to the structure of the particle's quantum phase space (QPS). The direct calculation from the relation (26) gives :

$$\frac{\partial \rho}{\partial t} = [\Phi(t) + i\Theta(t)]\rho(\langle z \rangle, \langle z' \rangle, t) \quad (27)$$

where

- For stationary environment (Markovian regime,  $\dot{\mathcal{G}} = 0$ )

$$\begin{cases} \Phi = \Phi_M = [-\frac{1}{4}\langle u_0 \rangle \mathcal{G}^{-1}(\langle y_0 \rangle + \langle y'_0 \rangle)] \\ \Theta = \Theta_M = \frac{1}{2\hbar}[\langle p_0 \rangle(\langle x \rangle - \langle x' \rangle) - \langle \dot{x}_0 \rangle(\langle p \rangle - \langle p' \rangle)] \end{cases} \quad \begin{aligned} \langle \dot{x}_0 \rangle &= \frac{d\langle x_0(t) \rangle}{dt} & \langle \dot{p}_0 \rangle &= \frac{d\langle p_0(t) \rangle}{dt} \end{aligned} \quad (28)$$

- For reactive environment (Non-Markovian regime,  $\dot{\mathcal{G}} \neq 0$ )

$$\begin{cases} \Phi = \Phi_{NM} = [-\frac{1}{8}[(\langle y_0 \rangle) \dot{\mathcal{G}}^{-1}(\langle y_0 \rangle)^T + (\langle y'_0 \rangle) \dot{\mathcal{G}}^{-1}(\langle y'_0 \rangle)^T] - \frac{1}{4}\langle u_0 \rangle \mathcal{G}^{-1}(\langle y_0 \rangle + \langle y'_0 \rangle)] \\ \Theta = \Theta_{NM} = \frac{1}{2\hbar}[\langle \dot{p}_0 \rangle(\langle x \rangle - \langle x' \rangle) - \langle \dot{x}_0 \rangle(\langle p \rangle - \langle p' \rangle)] \end{cases} \quad \begin{aligned} \dot{\mathcal{G}} &= \begin{pmatrix} \dot{\mathcal{P}} & \dot{\mathcal{Q}} \\ \dot{\mathcal{Q}} & \dot{\mathcal{X}} \end{pmatrix} & \text{and} & \dot{\mathcal{G}}^{-1} = -\mathcal{G}^{-1} \dot{\mathcal{G}} \mathcal{G}^{-1} & \langle u_0 \rangle &= (\langle \dot{p}_0 \rangle & \langle \dot{x}_0 \rangle) \end{aligned} \quad (29)$$

## 5.1 Identification in the Markovian regime

In the Markovian case, we may consider the Lindblad master equation [2, 8, 41, 42, 43]. This master equation can be written in the following form:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[\mathbf{H}, \rho] + \frac{1}{2\hbar} \sum_{j=1}^2 \left\{ [V_j \rho, V_j^\dagger] + [V_j, \rho V_j^\dagger] \right\} \quad (30)$$

where,

·  $\mathbf{H}$  is the particle Hamiltonian, we may consider the example of a general quadratic form

$$\mathbf{H} = A_{pp}(\mathbf{p})^2 + A_{xx}(\mathbf{x})^2 + A_{px}(\mathbf{x}\mathbf{p} + \mathbf{p}\mathbf{x}) + A_p\mathbf{p} + A_x\mathbf{x} + A \quad (31)$$

·  $\mathbf{V}_j, \mathbf{V}_j^\dagger$  are the operators which describe the interaction between the particle and its environment. We can consider, for instance, that these operators are linear functions of the momentum and position operators [2, 43]  $\mathbf{V}_j = a_j\mathbf{p} + b_j\mathbf{x}$  and the following coefficients are introduced :

$$\begin{cases} D_{xx} = \frac{\hbar}{2} \sum_{j=1}^2 |a_j|^2 \\ D_{pp} = \frac{\hbar}{2} \sum_{j=1}^2 |b_j|^2 \\ D_{px} = -\frac{\hbar}{2} \operatorname{Re} \sum_{j=1}^2 (a_j^* b_j) \\ \Lambda = -\operatorname{Im} \sum_{j=1}^2 (a_j^* b_j) \end{cases} \quad (32)$$

$D_{xx}$ ,  $D_{pp}$  and  $D_{px}$  are the diffusion coefficients and  $\Lambda$  is the friction coefficient. Using the relations (22), (27), (28), (30), (31) and (32) we can deduce the following identification

$$\begin{cases} \mathcal{P} = \frac{D_{pp}}{\Lambda} \\ \mathcal{X} = \frac{D_{xx}}{\Lambda} \\ \mathcal{Q} = \frac{D_{px}}{\Lambda} \end{cases} \quad \begin{cases} A_{pp} = \frac{1}{2m} \\ A_{xx} = \frac{\mathcal{P}}{2m\mathcal{X}} = \frac{1}{2m} \frac{D_{pp}}{D_{xx}} \\ A_{px} = -\frac{\mathcal{Q}}{2m\mathcal{X}} = -\frac{1}{2m} \frac{D_{px}}{D_{xx}} \\ A_P = -\dot{p}_0 \\ A_x = \dot{x}_0 \\ A : \text{arbitrary} \end{cases} \quad (33)$$

These relations explicitly describe the connections between the properties of the environment (characterized by the diffusion and friction coefficients) and the structure of the quantum phase space (described by the variance-covariance matrix) in the considered Markovian regime.

## 5.2 Identification in Non-Markovian regime

To account for environmental memory effects, we must adopt a non-Markovian master equation [8, 16, 44]:

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar} [\mathbf{H}_S, \rho(t)] + \mathcal{L}_{NM}[\rho(t)]. \quad (34)$$

For instance, the non-Markovian superoperator can be expressed as

$$\mathcal{L}_{NM}[\rho(t)] = \sum_{j=1}^2 \int_0^t d\tau \left( C_j(t-\tau) [\mathbf{V}_j, [\mathbf{V}_j(\tau-t), \rho(t)]] - i D_j(t-\tau) [\mathbf{V}_j, \{\mathbf{V}_j(\tau-t), \rho(t)\}] \right), \quad (35)$$

where

$$\tilde{V}_j(s) = e^{iH_S s/\hbar} V_j e^{-iH_S s/\hbar}. \quad (36)$$

The functions  $C_j(t)$  and  $D_j(t)$  represent the noise correlations and dissipation kernels of the environment. The diffusion and dissipation coefficients become time dependent:

$$D_{xx}(t) = \frac{\hbar}{2} \sum_{j=1}^2 \int_0^t d\tau C_j(\tau) |a_j|^2 \cos(\omega_j \tau), \quad (37)$$

$$D_{pp}(t) = \frac{\hbar}{2} \sum_{j=1}^2 \int_0^t d\tau C_j(\tau) |b_j|^2 \cos(\omega_j \tau), \quad (38)$$

$$D_{px}(t) = -\frac{\hbar}{2} \sum_{j=1}^2 \int_0^t d\tau C_j(\tau) \Re(a_j^* b_j) \cos(\omega_j \tau), \quad (39)$$

$$\Lambda(t) = - \sum_{j=1}^2 \int_0^t d\tau D_j(\tau) \Im(a_j^* b_j) \sin(\omega_j \tau). \quad (40)$$

The parameters defining the pointer states and the structure of the QPS are then

$$\mathcal{P}(t) = \frac{D_{pp}(t)}{\Lambda(t)}, \quad \mathcal{X}(t) = \frac{D_{xx}(t)}{\Lambda(t)}, \quad \mathcal{Q}(t) = \frac{D_{px}(t)}{\Lambda(t)}. \quad (41)$$

They always satisfy the minimum uncertainty condition

$$\mathcal{P}(t)\mathcal{X}(t) - \mathcal{Q}(t)^2 = \frac{\hbar^2}{4}. \quad (42)$$

## 6 Discussion and conclusion

This work has introduced and developed a novel theoretical framework grounded in Quantum Phase Space (QPS) to address the fundamental and practical challenges of quantum decoherence in nanoscience. Our approach unifies the dual pillars of the decoherence process: the dynamical selection of pointer states and the characterization of decoherence regimes. By connecting environmental properties to the geometry of phase space, we provide a powerful tool for modeling, analyzing, and potentially controlling quantum coherence at the nanoscale.

Our central achievement is the identification of pointer states for a particle's motional degrees of freedom as minimum-uncertainty states  $|\langle z \rangle\rangle$ , that saturate the uncertainty relation. This resolves the theoretical impasse presented by idealized position or momentum eigenstates, which are physically inadmissible under the uncertainty principle. These states, defined by their expectation values  $(\langle p \rangle, \langle x \rangle)$  and a given variance-covariance structure  $\mathcal{G} = \begin{pmatrix} \mathcal{P} & \mathcal{Q} \\ \mathcal{Q} & \mathcal{X} \end{pmatrix}$ , constitute the closest quantum analogue to a classical phase-space points. Consequently, they provide the natural, physically sound basis, the pointer basis, into which a system decoheres. The structure of the QPS, encoded in the matrix  $\mathcal{G}$  is not static but is directly shaped by the environment . We have demonstrated that this provides a unifying geometric criterion to distinguish decoherence regimes:

- The Markovian (stationary) regime: This corresponds to a memoryless, broadband environment whose statistical properties are unchanging. Within our framework, this is characterized by a time-independent variance-covariance matrix  $\dot{\mathcal{G}} = \frac{d\mathcal{G}}{dt} = \begin{pmatrix} \dot{\mathcal{P}} & \dot{\mathcal{Q}} \\ \dot{\mathcal{Q}} & \dot{\mathcal{X}} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ . By applying this condition within the Lindblad master equation formalism for a specific example, we derived explicit, closed-form relations (Eq. 32) showing how the diffusion and friction coefficients of the environment uniquely determine the fixed ellipsoid of uncertainty in phase space. This formalizes the concept that a stationary environment selects and "freezes" a specific set of quasi-classical trajectories.
- The Non-Markovian (reactive) regime: This describes environments with memory, structure, or strong coupling, where past interactions influence future dynamics. Here, the environment is reactive, and its statistical imprint on the system evolves. Mathematically, this is captured by a time-dependent variance-covariance matrix  $\mathcal{G}(t)$ . Using Non-Markovian master equation, we showed how time-dependent diffusion and friction coefficients (Eqs. 36-39) govern the evolution of  $\mathcal{G}(t)$  . This "breathing" or rotation of the uncertainty ellipse in phase space provides a direct geometric representation of non-exponential decoherence, recoherence, and information backflow.

A key strength of the QPS framework is its ability to seamlessly encompass both Markovian and non-Markovian dynamics within a single, consistent mathematical language . It transcends the traditional modeling dichotomy by showing that both regimes are manifestations of how environmental properties, encoded in spectral densities and correlation functions, imprint themselves onto the phase space geometry. The QPS framework offers a clear metric, the time-dependence of  $\mathcal{G}(t)$  to quantify non-Markovian memory. This can guide the active harnessing of environmental backaction for quantum advantage, such as using

structured environments for enhanced quantum sensing or leveraging memory effects in reservoir engineering for information processing.

In conclusion, our Quantum Phase Space framework turns the abstract problem of decoherence into a concrete, visual, and geometrically sound approach. By integrating the dynamics of pointer state selection and coherence decay into the evolving structure of the quantum phase space, this approach provides a powerful synthetic tool. It not only deepens our fundamental understanding of how quantum systems interact with their environments but may also deliver a practical and unified methodology for modeling, mitigating, and potentially harnessing decoherence, particularly in the fields of nanoscience and quantum technologies.

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