Preferred States of Decoherence under Intermediate System-Environment Coupling

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The notion that decoherence rapidly reduces a superposition state to an incoherent mixture implicitly adopts a special representation, namely, the representation of preferred (pointer) states (PS). For weak or strong system-environment coupling, the behavior of PS is well known. Via a simple dynamical model that simulates a two-level system interacting with few other degrees of freedom as its environment, it is shown that even for intermediate system-environment coupling, approximate PS may still emerge from the coherent quantum dynamics of the whole system in the absence of any thermal averaging. The found PS can also continuously deform to expected limits for weak or strong system-environment coupling. Computational results are also qualitatively explained. The findings should be useful towards further understanding of decoherence and quantum thermalization processes.

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Introduction — As illustrated by the Schrödinger cat paradox, there is a clash between the quantum superposition principle and the way we perceive the macroscopic reality. So how does a classical world emerge from the quantum? One promising solution to this profound question is decoherence, i.e., the loss of quantum coherence due to the interaction of a system of interest with its environment [1–3]. Decoherence may rapidly reduce a coherent superposition state of the system to an incoherent mixture. During this process the environment singles out special basis states, often called “preferred (pointer) states” (PS), of which a classical probabilistic description becomes sufficient to describe the system and the bizarre superposition state of the PS is out of the picture. That is, in the PS representation the reduced density matrix (RDM) of the system becomes diagonal as time evolves.

Such a decoherence perspective is not expected to resolve all conceptual issues regarding quantum weirdness vs classical reality. Nevertheless, it is highly useful as it implies the environment-dependence of the quantum-classical transition and the representation-dependent nature of decoherence issues. For example, different environments may select different PS, and a quantum system decohered in one PS representation may still possess certain quantum coherence in other representations. Going further, one may envision the possibilities of environment engineering to form desired PS [4], such that system properties are robust to decoherence.

PS have been identified in several cases. If the system-environment interaction is in the adiabatic limit or if it commutes with the system’s self-Hamiltonian, then popu-
states of the system-environment interaction Hamiltonian, undergo continuous deformation as the system-environment coupling strength varies. These findings show that decoherence-induced superselection rule can be twofold: superposition states of the PS are destroyed but PS themselves can be rich superposition states for intermediate system-environment coupling. Equally interesting, it can be concluded that the concept of PS is still important in understanding quantum dynamical processes in the absence of any thermal averaging.

**Identifying PS from the time-evolving RDM** — If PS exists, then the RDM will gradually become diagonal in the PS representation. On the other hand, the same RDM is always diagonal in its own eigenrepresentation. Therefore, if we computationally track the eigenstates of the RDM, then we can see clearly whether or not a well-defined set of PS can emerge from a decoherence process. That is, if after a certain period the eigenstates of the RDM are found to evolve closely around a fixed basis set, then this fixed set of states can be defined as the PS, at least approximately. This computational definition of PS extends the PS criterion used by Diósi and Kiefer [8]. Note also that such a definition of PS gives up their precise analytical form. Consistent with this picture, the off-diagonal elements of the RDM in the PS representation must be also small when compared with the difference of its diagonal elements. Indeed, were the RDM diagonal elements almost degenerate, then a small fluctuation in the off-diagonal elements can still cause a drastic rotation of the RDM eigenstates, a fact that would contradict with the existence of PS [18]. We hence mainly work in the parameter regimes where an appreciable difference between the diagonal elements of RDM can emerge from the dynamics. These preliminaries also make it clear that even a stationary RDM does not necessarily mean the existence of PS.

Consider now a two-level system $S$ interacting with its environment $E$, with a total Hamiltonian $H = H_S + H_I + H_E$, where $H_S$ and $H_E$ are the Hamiltonians of $S$ and $E$, and $H_I$ is the system-environment interaction Hamiltonian, with $[H_S, H_I] \neq 0$. Eigenstates of $H_S$ are denoted by $|E_k\rangle$, with $k = 0, 1$. Throughout, we use $|\Psi\rangle$ to denote a state vector for the whole system-environment configuration, denoted by $S + E$ and isolated from any thermal bath. The time-evolving RDM for $S$ is given by $\rho_S(t) \equiv \text{Tr}_E (|\Psi(t)\rangle \langle \Psi(t)|)$, where $|\Psi(t)\rangle = e^{-iHt/\hbar} |\Psi(0)\rangle$ coherently evolves according to Schrödinger equation for $S + E$.

Eigenstates of the RDM $\rho_S(t)$ are represented by $|\rho_k(t)\rangle$, with eigenvalues $\rho_k(t)$, i.e., $\rho^* (t) |\rho_k(t)\rangle = \rho_k(t) |\rho_k(t)\rangle$. The two states $|\rho_0(t)\rangle$ and $|\rho_1(t)\rangle$ also form an orthonormal basis set for the Hilbert subspace associated with $H_S$. The distance between this basis set and another basis set $|\eta_{k'}\rangle$ ($k' = 0, 1$) for the same subspace may be measured by $D(|\rho_k(t)\rangle, |\eta_{k'}\rangle) = 1 - |\langle \rho_k(t)|\eta_{k'}\rangle|^2$, with $k$ and $k'$ determined by the condition $|\langle \rho_k|\eta_{k'}\rangle|^2 \geq 1/2$. A time-averaged distance $d$ over a period $[t_a, t_b]$ can then be defined as $d(|\eta_{k'}\rangle) = \int_{t_a}^{t_b} dt' \; D(|\rho_k(t')\rangle, |\eta_{k'}\rangle)$. If, for a particular basis set $\{ |\rho_k\rangle \}$ defined below, $d(|\rho_k\rangle)$ is small for sufficiently large $t_a, t_b$, and $t_b - t_a$, then $\rho(t)$ becomes almost diagonal in the $\{ |\rho_0\rangle, |\rho_1\rangle \}$ representation, and hence $\{ |\rho_0\rangle, |\rho_1\rangle \}$ can be computationally identified as the PS.

To find $\{ |\rho_0\rangle, |\rho_1\rangle \}$ that may reflect the average behavior of $|\rho_k(t)\rangle$ with acceptable fluctuations, we calculate the time-evolving RDM eigenstates $|\rho_k(t)\rangle$, average the density matrix $|\rho_k(t)\rangle \langle \rho_k(t)|$ over time (value of $k = 0$ or $k = 1$ is chosen to maintain a continuity), and then obtain a time-averaged density matrix $\overline{\rho}$. Finally, the eigenstates of $\overline{\rho}$ are defined as the basis states $\{ |\rho_0\rangle, |\rho_1\rangle \}$. If, in the $\{ |\rho_0\rangle, |\rho_1\rangle \}$ representation, $|\rho_0(t)\rangle \ll |\rho_{00}(t) - \rho_{11}(t)|$ for sufficiently large times $t$, then $d(|\rho_k\rangle)$ is small and PS can hence be identified [19]. If this is not the case, then PS fails to emerge from the dynamics.

**Model** — We now turn to a concrete model. To reflect the fact that typically a small system $S$ is not directly coupled to the whole of its environment $E$, we let $S$ be directly coupled to a small component $A$ of $E$, and then let $A$ be further coupled to the rest part $B$ of $E$, with $E = A + B$. For convenience, $A$ is also assumed to be a two-level system. Such kind of coupling scheme was also considered recently [20] to model a nonlinear system-environment coupling. It can be also qualitatively argued that our coupling scheme can yield much less fluctuation in the RDM than a full coupling between $S$ and $E$ does. The $B$ part of $E$ is simulated by a quantum kicked rotor on a torus with only 1 degree of freedom, whose classical limit is fully chaotic [21, 22]. The irregular motion of $B$ due to quantum chaos, instead of many noninteracting degrees of freedom of a thermal bath, is responsible for decoherence in $S$. In terms of standard Pauli matrices and operators for a kicked rotor in dimensionless units, the Hamiltonians for the system, the environment, and their coupling are

$$
H_S = \omega_x \sigma_x^S + \omega_z \sigma_z^S, \quad H_I = \varepsilon \sigma_x^A \otimes \sigma_z^S,
$$

$$
H_E = H_A + H_B + H_{AB}.
$$

(1)

Here, $H_A = \omega_A \sigma_x^A$, $H_B = \frac{p^2}{2} + \hbar \cos \gamma \sum_j \delta(t - j T)$, and $H_{AB} = \lambda \sigma_x^A \cos \gamma \sum_j \delta(t - j T)$, where $p$ and $\gamma$ are momentum and coordinate operators of the kicked rotor. Since the system-environment coupling is already of the $\sigma_x^A$ type, for generality $H_S$ is made to contain both $\sigma_x^A$ and $\sigma_z^A$ terms [24]. The unitary propagator associated with one period $T$ is (with $h = 1$).

$$
\hat{U}_T = e^{-i T (\omega_x \sigma_x^S + \omega_z \sigma_z^S + \omega_A \sigma_x^A + \epsilon \sigma_x^A \otimes \sigma_z^S)} \\
\times e^{-i T \frac{p^2}{2} - i \hbar \cos \gamma e^{-i \lambda \sigma_x^A \cos \gamma}.}
$$

(2)

The initial state is chosen as $|\Psi(0)\rangle = |\psi^S_0\rangle \otimes |\varphi_0\rangle_A \otimes |\varphi_0\rangle_B$, where $|\psi^S_0\rangle$ and $|\varphi_0\rangle_B$ are vectors in the Hilbert spaces of
S of and \( B \), and \(|0\rangle_A \) is an eigenstate of \( H_A \). The quantum kicked rotor is quantized on a phase space torus with a Hilbert space dimension \( N = 4096 \), whose initial state is taken as a randomly generated vector from its Hilbert space (quantum recurrence time is already sufficiently large). The kicking period \( T \) is taken as \( 2\pi/N \). Typical values of \( \omega_x \), \( \omega_z \), and \( \omega_A \) are set around \( 10^3 \) in dimensionless units, such that within one kicking period \( T \) the characteristic phase evolution of the two-level systems are of the order of unity. Many initial states were studied but in Fig. 1 we only report representative results for one initial state. Note also that one key parameter is \( \varepsilon \), which represents the strength of system-environment coupling.

As shown in Ref. [11], if the system-environment coupling strength \( \varepsilon \) is below a threshold \( \varepsilon_p \), then the off-diagonal elements of the RDM in the eigenrepresentation of \( H_S \) will show a Gaussian-type decay. The dephasing time of energy eigenstates \( (T_2) \) then scales as \( \varepsilon^{-1} \), whereas the population relaxation time \( (T_1) \) goes as \( \varepsilon^{-2} \) (obtained from Fermi’s golden rule). In our model we find \( \varepsilon_p \sim 1/N \). So for \( \varepsilon < 1/N \), \( T_2 \ll T_1 \), and hence the energy eigenstates \( |E_k\rangle \) form the PS. Detailed calculations from our present model confirm this and also reveal something interesting. As shown in Fig. 1 (empty squares), \( |E_k\rangle \) are found to agree well with the computationally found PS (i.e., very small values of \( \theta \)) as \( \varepsilon \) as large as \( 10^4 \). Though our previous work [11] did not rule out the possibility of \( |E_k\rangle \) being the PS for \( \varepsilon > \varepsilon_p \), it is remarkable to see that \( |E_k\rangle \) here still form the PS even for \( \varepsilon \gg \varepsilon_p \). This should be related to the fact that here the system \( (S) \) is only directly coupled with a small component \( (A) \) of the environment.

Results for larger values of \( \varepsilon \) are also detailed in Fig. 1. Consider first \( \varepsilon \) values approaching \( 10^3 \), i.e., the right end of the curve shown with empty triangles. In these cases, the computationally found states \( |\tilde{\rho}_k\rangle \) are rotated from the \( H_I \) eigenstates by essentially a zero angle. Hence, the eigenstates of \( H_I \) can be regarded as the PS in this strong coupling case, even for a time scale much larger than the characteristic scale of \( H_S \). Next we turn to intermediate cases with \( \varepsilon \in [10^2, 5 \times 10^3] \). As seen from Fig. 1, states \( |\tilde{\rho}_k\rangle \) can notably deviate from \( |E_k\rangle \) as well as the \( H_I \) eigenstates. As we tune up the value of \( \varepsilon \), states \( |\tilde{\rho}_k\rangle \) exhibit a clear and smooth transition from being close to \( |E_k\rangle \) to being close to the \( H_I \) eigenstates. Further, as a consistency check, the inset of Fig. 1 shows the decay of the off-diagonal elements of the RDM in three representations, for \( \varepsilon = 2000 \) as an example. It is seen that only in the \( |\tilde{\rho}_k\rangle \) representation, the off-diagonal elements decay to small values with some fluctuations [24].
It is yet to be shown that at sufficiently later times the eigenstates \(|\rho_k(t)\rangle\) of the time-evolving RDM only slightly fluctuate around \(|\tilde{\rho}_k\rangle\). The upper panel of Fig. 2 depicts the distance \(d(|\rho_0(t)\rangle)\) vs \(\varepsilon\) (solid line) (i.e., for the PS identified in Fig. 1). It is seen that for the entire considered regime of \(\varepsilon\), \(d\) remains impressively small. For intermediate values of \(\varepsilon\), it is much smaller than the same \(d\)-distance between \(|\rho_0(t)\rangle\) and eigenstates of \(H_S\) (dashed red line) or between \(|\rho_0(t)\rangle\) and eigenstates of \(H_I\) (dotted blue line). Therefore, after an initial period the time-evolving RDM eigenstates \(|\rho_0(t)\rangle, |\rho_1(t)\rangle\) remain close to \(|\tilde{\rho}_0\rangle, |\tilde{\rho}_1\rangle\), suggesting that the RDM becomes almost diagonal in the \(|\tilde{\rho}_k\rangle\) representation, even for intermediate values of \(\varepsilon\). We finally infer that the states \(|\tilde{\rho}_k\rangle\), whose behavior is shown in Fig.1, are indeed excellent PS emerging from the coherent quantum dynamics of \(S + E\). Other detailed calculations also indicate that PS does not always exist. For example, if the coupling between \(A\) and \(B\) is also very strong (e.g., \(\lambda = 1.0\), bottom panel of Fig. 2), then the diagonal elements of RDM become very close, \(d\) can reach as large as 0.25 (dashed line) (a value that can be estimated theoretically \([18]\)), and consequently PS is lost.

**Theoretical insights** — We shall now develop some insights into our computational results. We rewrite the total state for \(S + E\) as

\[
|\Psi(t)\rangle = |\alpha\rangle|\phi_\alpha(t)\rangle + |\beta\rangle|\phi_\beta(t)\rangle,
\]

where \(|\alpha\rangle, |\beta\rangle\) is a chosen time-independent orthonormal basis set in the Hilbert subspace for \(S\), \(|\phi_\alpha(t)\rangle\) and \(|\phi_\beta(t)\rangle\) are the associated “expansion states” living in the Hilbert subspace for \(E\). The time-dependence of the off-diagonal element of the system’s RDM is then given by

\[
\rho_{\alpha\beta}^s(t) \equiv \langle \alpha|\rho^s(t)|\beta\rangle = \langle \phi_\beta(t)|\phi_\alpha(t)\rangle.
\]

With this notation, seeking PS then becomes the search for \(|\rho_{\alpha\beta}(t)\rangle\), such that the evolution of \(|\phi_\alpha(t)\rangle\) is as different as possible from \(|\phi_\beta(t)\rangle\). This insight motivates us to examine the time evolution of the states \(|\phi_\alpha(t)\rangle\) and \(|\phi_\beta(t)\rangle\) used in Eq. (3). To that end, we first define \(H^S_{\alpha\beta} \equiv \langle \alpha|H S|\beta\rangle\), \(H^I_{\alpha\beta} \equiv \langle \alpha|H I|\beta\rangle\) (and those by \(\alpha \leftrightarrow \beta\)). Note that \(H^S_{\alpha\beta}\) thus defined is a scalar, but \(H^I_{\alpha\beta}\) is still an operator on the Hilbert subspace for \(E\). Just to have a rather compact Schrödinger-like equation for \(|\phi_\alpha(t)\rangle\) and \(|\phi_\beta(t)\rangle\), we introduce more operators on the \(E\) subspace, i.e., \(\Delta H^S \equiv H^E + H^1_{\alpha\alpha} + H^S_{\alpha\alpha}, H_{\alpha\beta} \equiv H^S_{\alpha\beta} + H^I_{\alpha\beta}, K_{\alpha} \equiv H_{\alpha\beta} H_{\beta\alpha}^{-1},\) and \(J_{\alpha} \equiv H_{\alpha\beta} H_{\beta\alpha}\). Using these definitions and the Schrödinger equation for \(S + E\), we obtain

\[
\frac{d}{dt}|\alpha\rangle = H_{\alpha\alpha}|\alpha\rangle + i|\xi_\alpha\rangle,
\]

where \(|\xi_\alpha\rangle = -iH_{\alpha\beta}|\phi_\beta\rangle\), with

\[
\frac{d}{dt}|\xi_\alpha\rangle = K_{\alpha}|\xi_\alpha\rangle - iJ_{\alpha}|\phi_\alpha\rangle.
\]

An analogical equation for \(|\phi_\beta(t)\rangle\) is obtained by exchanging \(\alpha\) and \(\beta\).

Equation (7) indicates that the difference between the evolution of \(|\phi_\alpha(t)\rangle\) and that of \(|\phi_\beta(t)\rangle\) is caused by the difference between the operators \(H_{\alpha\alpha}\) and \(H_{\beta\beta}\) and by the difference between \(|\xi_\alpha\rangle\) and \(|\xi_\beta\rangle\). Further, Eq. (8) shows that \(|\xi_\alpha\rangle\) and \(|\xi_\beta\rangle\) evolve differently due to the difference between \(K_{\alpha}\) and \(K_{\beta}\) and between \(J_{\alpha}\) and \(J_{\beta}\). To quantify these operator differences we define \(\Delta H \equiv H_{\alpha\alpha} - H_{\beta\beta}, \Delta K \equiv K_{\alpha} - K_{\beta},\) and \(\Delta J \equiv J_{\alpha} - J_{\beta}\). In our model, because \(H_I\) is a direct product of two spin operators, one finds \(\Delta J = 0\) \([18]\). Furthermore, for \(\varepsilon\) much less or much larger than the energy scale of \(H_S\), we find \(\Delta K \approx -\Delta H\) \([18]\). For cases with intermediate values of \(\varepsilon\), a more detailed analysis \([18]\) gives again that \(\Delta K \approx -\Delta H\), at least for those states \((|\alpha\rangle, |\beta\rangle)\) that maximize \(||\Delta H||\), where \(||\Delta H||\) represents the Frobenius-2 norm, a simple measure of \(\Delta H\). Putting these observations together, we intuitively expect (not a proof) that for the entire considered regime of \(\varepsilon\), the basis states \((|\alpha\rangle, |\beta\rangle)\) maximizing \(||\Delta H||\) may approximately give the most substantial difference between \(|\phi_\alpha(t)\rangle\) and \(|\phi_\beta(t)\rangle\) and hence the most significant decay of \(|\rho_{\alpha\beta}^s(t)\rangle\). As such, the basis states \((|\alpha\rangle, |\beta\rangle)\) theoretically determined by maximizing \(||\Delta H||\) should agree with the PS computationally obtained above.

In Fig.1 we compare the PS (empty symbols) found from the decoherence dynamics with the states \((|\alpha\rangle, |\beta\rangle)\) (filled symbols) determined directly by maximizing \(||\Delta H||\). In terms of their relation with the eigenstates of \(H_S\) and of \(H_I\), nice agreement is obtained for the whole regime of \(\varepsilon\).

It is also interesting to discuss the implication of the term \(i|\xi_\alpha\rangle\) in Eq. (7). Note that this term does not preserve the norm \(|\phi_\alpha(t)\rangle\). Hence, populations on the basis states \((|\alpha\rangle, |\beta\rangle)\), even when they are identified as the PS, can still fluctuate with time. This constitutes a crucial difference from a pure-dephasing problem. Unlike in a pure-dephasing problem, here the decay of \(\rho_{\alpha\beta}^s = \langle \phi_\beta(t)|\phi_\alpha(t)\rangle\) cannot be interpreted as that of the overlap of two independent environment histories \(|\phi_\alpha(t)\rangle\) and \(|\phi_\beta(t)\rangle\). Instead, these two evolution histories are mingled together through population transitions between them. Difference from a pure-dephasing picture is also made evident by the role of the term \(\Delta H^S \equiv H^S_{\alpha\alpha} - H^S_{\beta\beta}\) as one component of \(\Delta H = \Delta H^S + H^I_{\alpha\alpha} - H^I_{\beta\beta}\). For a pure-dephasing problem, i.e., if the term \(i|\xi_\alpha\rangle\) is switched off, then the component \(\Delta H^S\) becomes irrelevant: it is a c-number for the environmental Hilbert subspace, and hence cannot cause the decay of \(|\langle \phi_\beta(t)|\phi_\alpha(t)\rangle\). By contrast, in our model the term \(\Delta H^S\) in \(\Delta H\) is found to be necessary for predicting the PS with intermediate system-environment coupling. That is, without this term, maximization of \(||\Delta H||\) would incorrectly predict that eigenstates of \(H_I\) are the PS regardless of the value of \(\varepsilon\).
Conclusion — The concept of PS may still apply if an environment with many degrees of freedom (like a thermal bath) is replaced by an environment with very few degrees of freedom. Approximate PS are shown to exist for intermediate system-environment coupling and can continuously deform to expected limits. Such types of PS emerging from quantum dynamics alone are of importance to understanding decoherence and thermalization processes.

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[18] See supplementary material accompanying this submission for discussions on conditions for PS to be identified computationally, for a distance $d$ obtained by averaging over the Hilbert space, and for a detailed analysis in properties of $\Delta H$, $\Delta K$, and $\Delta J$ in the model studied in this paper.
[19] Certainly this convention is just one possibility for picking out a good reference basis set $\{|\tilde{\rho}_0\rangle, |\tilde{\rho}_1\rangle\}$ to which the time-evolving states $|\rho_{\alpha}(t)\rangle$ will be compared. What really matters here is whether PS can be found, i.e., whether the eigenstates of the RDM can indeed stay close to some time-independent basis states.
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[23] If $\omega_\alpha = 0$, then $H_S$ is quantized along $z$ and $H_I$ is quantized along the perpendicular direction $z$. For this case, it was found that fluctuations around the computed intermediate PS are much larger due to close diagonal elements of the reduced density matrix.
[24] Because both pointer states were found to have appreciable populations (with populations around 0.4 and 0.6 in the case of the inset of Fig.3), they are not at all fixed-point solutions of the dynamics.

Supplementary Materials I: Some operators and equations used in the manuscript

To qualitatively understand the emergence of preferred (pointer) states (PS) for intermediate strength of system-environment coupling, we first recapitulate some equations and operators defined in our manuscript. In particular, the “expansion states” living in the Hilbert subspace of the environment is denoted by $|\phi_\alpha(t)\rangle$, with $\{|\phi_\alpha(t)\rangle + |\beta\rangle\phi_\beta(t)\rangle$, where $\{|\alpha\rangle, |\beta\rangle\}$ is an intermediate orthonormal basis set in the Hilbert subspace of the system $S$.

Using Schrödinger equation for the system and the environment as a whole, under the condition that $H_{\alpha\beta}$ does not explicitly depend on the time $t$ and is a reversible operator, the equation of motion of $|\phi_\alpha(t)\rangle$ is given by

$$i\frac{d}{dt}|\phi_\alpha\rangle = H_{\alpha\alpha}|\phi_\alpha\rangle + i|\xi_\alpha\rangle,$$

$$\frac{d}{dt}|\xi_\alpha\rangle = K_\alpha|\xi_\alpha\rangle - iJ_\alpha|\phi_\alpha\rangle,$$

where

$$H_{\alpha\alpha} = H_E + H_{I\alpha}^I + H_S^I,$$

$$K_\alpha = H_{\alpha\beta}H_{\beta\alpha}^{-1},$$

$$J_\alpha = H_{\alpha\beta}H_{\beta\alpha},$$

with

$$H_{\alpha\beta} = H_S^I + H_{I\alpha}^I,$$

$$H_{\alpha\beta}^I = \langle\alpha|H_S^I|\beta\rangle,$$

$$H_{\alpha\beta} = \langle\alpha|H_I^I|\beta\rangle,$$

and analogous expressions by exchanging $\alpha$ and $\beta$. In the manuscript we then defined the following operators:

$$\Delta H = H_{\alpha\alpha} - H_{\beta\beta},$$

$$\Delta K = K_\alpha - K_\beta,$$

$$\Delta J = J_\alpha - J_\beta.$$
The vector $|\xi_0\rangle$ is in fact related to $|\phi_\beta\rangle$ by $|\xi_0\rangle = -iH_{\alpha\beta}|\phi_\beta\rangle$. For an initial system-environment direct-product state $|\Psi(0)\rangle = |\psi_S^0\rangle|\phi_0\rangle$, we have $|\phi_\alpha(0)\rangle = (\langle\alpha|\psi_S^0\rangle)|\phi_0\rangle$ and $|\phi_\beta(0)\rangle = (\langle\beta|\psi_S^0\rangle)|\phi_0\rangle$. Thus, the initial condition of Eqs. (7) and (8) is given by $|\phi_\alpha(0)\rangle$ and $|\xi_0(0)\rangle = -i(\langle\beta|\psi_S^0\rangle)H_{\alpha\beta}|\phi_0\rangle$.

Note that $\langle\phi_\alpha(t)|\phi_\alpha(t)\rangle$ and $\langle\phi_\beta(t)|\phi_\beta(t)\rangle$ give the probabilities of finding the system in the states $|\alpha\rangle$ and $|\beta\rangle$, respectively. During the time evolution, these two quantities need not to be conserved because the problem of interest here is not a pure-dephasing problem.

**Supplementary Materials II: On conditions for PS to be identified computationally**

In our manuscript we also mentioned conditions under which we can computationally identify PS from the time-evolving reduced-density matrix (RDM) of the system. These conditions are further elaborated in this section. After some simple derivation, we obtain the following expression for the distance $D(|\rho_k(t), |\alpha\rangle) = 1 - |\langle\rho_k(t)|\alpha\rangle|^2$, where the eigenstate $|\rho_k(t)\rangle$ of the RDM $\rho^s(t)$ is chosen by the condition $|\langle\rho_k(t)|\alpha\rangle|^2 \geq 1/2$,

$$D(|\rho_k(t), |\alpha\rangle) = \frac{|\rho^s_{\alpha\beta}|^2}{\frac{1}{4} \left[ \delta\rho + \sqrt{(\delta\rho)^2 + 4|\rho^s_{\alpha\beta}|^2} \right]^2 + |\rho^s_{\alpha\beta}|^2}. \quad (12)$$

Here, $\delta\rho \equiv |\rho^s_{\alpha\alpha} - \rho^s_{\beta\beta}|$, with $\rho^s_{\alpha\alpha}$ ($\rho^s_{\beta\beta}$) being the diagonal (off-diagonal) matrix elements of the RDM. The time-averaged value of $D(|\rho_k(t), |\alpha\rangle)$ is denoted by $d(|\alpha\rangle)$ in the manuscript.

Suppose at long times, the overlap $\langle\phi_\beta(t)|\phi_\alpha(t)\rangle$ is already of a small magnitude. Then, $\rho^s_{\alpha\beta} = \langle\phi_\beta(t)|\phi_\alpha(t)\rangle$ is small by definition. Furthermore, we assume that the populations in the two basis states, namely, $\rho^s_{\alpha\alpha}$ and $\rho^s_{\beta\beta}$, have also approached some equilibrium values at long times and can maintain an appreciable difference $\delta\rho$ such that $\delta\rho \gg |\rho^s_{\alpha\alpha}|$. Then, Eq. (12) becomes

$$D(|\rho_k(t), |\alpha\rangle) \approx \frac{|\rho^s_{\alpha\beta}|^2}{(\delta\rho)^2}. \quad (13)$$

This then gives

$$d(|\alpha\rangle) \approx \left[ \frac{1}{t_b - t_a} \int_{t_a}^{t_b} |\rho^s_{\alpha\beta}|^2 dt \right] \frac{1}{(\delta\rho)^2} \ll 1. \quad (14)$$

Sufficiently small value of $d(|\alpha\rangle)$ indicates that eigenstates of the RDM $\rho^s(t)$ only have small fluctuations around the fixed set of basis $\langle|\alpha\rangle, |\beta\rangle\rangle$. This fixed set of basis states then form the PS, at least approximately.

In our manuscript we computationally identified such a basis set, which is denoted by $|\tilde{\rho}_k\rangle$.

It is now clear that PS can be computationally identified under the following conditions: (1) small $|\rho^s_{\alpha\beta}|$ and (2) relatively large $\delta\rho$. Smallness of $|\rho^s_{\alpha\alpha}|$ is equivalent to the smallness of the overlap $\langle|\phi_\beta(t)|\phi_\alpha(t)\rangle$. This occurs if $\Delta H$, $\Delta K$, and $\Delta J$ are made as different as possible, because these operators will determine the evolution difference between $|\phi_\beta(t)\rangle$ and $|\phi_\alpha(t)\rangle$.

**Supplementary Materials III: Distance $d$ averaged over the Hilbert space**

In the case of the bottom panel of Fig.2, the environment part $A$ is also strongly coupled with the kicked rotor, the distance $d$ is large and hence the PS is lost. Here we give a simple explanation. Due to the strong coupling within the environment and the strong coupling between $S$ and $E$, we can assume that the motion is sufficiently random in the total Hilbert space for $S + E$. Therefore, the long-time-averaged $d$ can be approximated by a Hilbert space average. Let $\langle d \rangle$ denote this total-Hilbert-space-averaged distance describing the difference between RDM eigentates and a fixed set of basis states $\langle|\alpha\rangle, |\beta\rangle\rangle$. In the following, we estimate $\langle d \rangle$ using a method similar to the canonical typicality approach discussed in Ref. [1]. The dimension of the Hilbert subspace of the environment $E$ is denoted by $n_E$ and the dimension of $S + E$ is $2n_E$.

Assuming that the dynamics is almost ergodic on the total Hilbert space, a “typical” vector in the total Hilbert space can be written as $|\Psi\rangle = \mathcal{N} \sum_{\alpha} |\alpha\rangle|\Phi^E_\alpha\rangle$, with $|\Phi^E_\alpha\rangle = \sum_j C_{\alpha j} |j\rangle$, (15) where $\{|j\rangle\}$ is an orthonormal basis set in the Hilbert subspace for the environment $E$, $\mathcal{N}$ is the normalization coefficient,

$$\mathcal{N} = \frac{1}{\sqrt{\sum_{\alpha j} |C_{\alpha j}|^2}} \approx \frac{1}{2n_E}, \quad (16)$$

and the real and imaginary parts of $C_{\alpha j}$ are assumed to be independent real Gaussian random variables with mean zero and variance 0.5. For this typical vector, the elements of the RDM are given by

$$\rho^s_{\alpha\beta} = \mathcal{N}^2 \sum_j C^*_{\beta j} C_{\alpha j}, \quad (17)$$

$$\delta\rho = |\rho^s_{\alpha\alpha} - \rho^s_{\beta\beta}| = \mathcal{N}^2 \left| \sum_j |C_{\alpha j}|^2 - |C_{\beta j}|^2 \right|. \quad (18)$$

In the limit of large $n_E$, after simple derivation one finds

$$\lim_{n_E \to \infty} \frac{\langle |\rho^s_{\alpha\beta}|^2 \rangle}{\langle (\delta\rho)^2 \rangle} = \frac{1}{2}, \quad (19)$$

with the average $\langle \cdot \rangle$ taken over all typical vectors defined above. Furthermore, using Eq. (12), one obtains that $\langle d \rangle = 0.25$, a result consistent with the bottom panel of Fig. 2. This clearly shows that PS does not always exist.
Supplementary Materials IV: Analysis of $\Delta H$, $\Delta K$, and $\Delta J$

Finally, we discuss how the three difference operators $\Delta H$, $\Delta K$, and $\Delta J$ may be used to predict PS without actually following the decoherence dynamics computationally. The qualitative picture is that in the PS representation, the operators $\Delta H$, $\Delta K$, and $\Delta J$ should be maximized such that the two evolution histories $|\phi_\beta(t)\rangle$ and $|\phi_\alpha(t)\rangle$ are as different as possible and hence the off-diagonal elements of the RDM will decay to very small values. Because in our model, $H_1$ has a product form, namely, $H_1 = \varepsilon \sigma_x^A \otimes \sigma_z^A$, we have

$$[H_{\beta\alpha}^I, H_{x\beta}^I] = 0, \quad (20)$$
$$\Delta J = H_{\alpha\beta}H_{\beta\alpha} - H_{x\alpha}H_{x\beta} = 0. \quad (21)$$

Given $\Delta J = 0$, we focus only on the maximization of $\Delta H$ and $\Delta K$ to understand the emergence of PS.

Interestingly, the two operators $\Delta H$ and $\Delta K$ are also related to each other. Let $X_\alpha = [H_{\alpha\beta}, H_\beta^I]$. Next, to have explicit expressions of operators, we now take the eigenstates of $\sigma_x$ as our working representation, where $|1\rangle_x$ and $|0\rangle_x$ represent spin up and down along the $x$-axis. We expand a given set of basis states $\{|\alpha\rangle, |\beta\rangle\}$ as the following:

$$|\alpha\rangle = a e^{i\varphi}|1\rangle_x + b|0\rangle_x,$$
$$|\beta\rangle = b e^{i\varphi}|1\rangle_x - a|0\rangle_x,$$  

where $a, b \in [0, 1]$ are real expansion coefficients. Using these two explicit expressions and our direct product form of $H_I$, we find

$$X_\alpha = [(1 - 2b^2)\sin(\varphi) + i \cos(\varphi)](2i\varepsilon \sigma_A^A) \sigma_y^A \quad (25)$$

and

$$Y = 2i \varepsilon \sigma_A^A \eta (L - \eta L), \quad (26)$$

where $\sigma_y^A$ is the Pauli operator along the $y$-axis for the two-level system $A$ as a part of the environment,

$$\eta = \frac{c_1}{d_1^2 - \varepsilon^2 c_1^2}, \quad \overline{\eta} = \frac{c_2}{d_2^2 - \varepsilon^2 c_2^2},$$
$$c_1 = (1 - 2b^2)\sin(\varphi) + i \cos(\varphi), \quad c_2 = c_1, \quad d_2 = d_1^*,$$  

and

$$L = -i\varepsilon c_1 \sigma_x^A + d_1 \sigma_y^A, \quad \overline{L} = -i\varepsilon c_2 \sigma_x^A + d_2 \sigma_y^A. \quad (28)$$

Let us consider the first limiting case of $\varepsilon \ll \omega_x$. Neglecting terms of the order of $\varepsilon/\omega_x$ and noticing that $\omega_i$ ($i = x, z, A$) are of the same order of magnitude, we find

$$\eta \simeq \frac{c_1}{d_1}, \quad \overline{\eta} \simeq \frac{c_2}{d_2}$$

$$L \simeq d_1 \sigma_y^A, \quad \overline{L} \simeq d_2 \sigma_y^A. \quad (29)$$

Thus,

$$Y \simeq 2i \varepsilon \left(\frac{\omega_A c_1}{d_1} - \frac{\omega_A c_2}{d_2}\right) \sigma_y^A \sim \varepsilon. \quad (30)$$

Clearly then, because $\Delta H \sim \omega_x$, one infers that $\Delta K \simeq -\Delta H$.

In the second limiting case of $\varepsilon \gg \omega_x$, we neglect all terms of the order of $\omega_x/\varepsilon$ and then obtain

$$\eta \simeq -\frac{1}{\varepsilon^2 c_1}, \quad \overline{\eta} \simeq -\frac{1}{\varepsilon^2 c_2}$$

$$L \simeq -i\varepsilon c_1 \sigma_x^A, \quad \overline{L} \simeq -i\varepsilon c_2 \sigma_x^A. \quad (31)$$

Thus,

$$Y \simeq 2\omega_A \sigma_x^A - 2\omega_A \sigma_x^A = 0. \quad (32)$$

This also leads us to the expectation that $\Delta K \simeq -\Delta H$. That is, for very small or very large system-environment coupling strength $\varepsilon$, we always have $\Delta K \simeq -\Delta H$.

The situation of intermediate system-environment coupling strength with $\varepsilon \sim \omega_x$ is more complicated. To better understand this case we have performed numerical calculations of the ratio,

$$r(\varepsilon, |\alpha\rangle) = \frac{\|Y\|}{\|\Delta H\|}. \quad (33)$$

![FIG. 3: Variation of the ratio $r$ with $\varepsilon$ for an arbitrarily chosen basis $|\alpha\rangle, |\beta\rangle$. Parameters: the same as in Fig. 1 of the text.](image)
FIG. 4: Variation of the ratio $r$ with $\varepsilon$ for the basis $(|\alpha\rangle, |\beta\rangle)$ that maximizes the norm $\|\Delta H\|$.

where $\|\ldots\|$ indicates a Frobenius-2 norm. Figure 1 shows the dependence of the ratio $r$ on $\varepsilon$ for an arbitrarily chosen basis $(|\alpha\rangle, |\beta\rangle)$. It shows that the ratio can be large for intermediate values of $\varepsilon$. Therefore, $\Delta K$ may have considerable deviations from $-\Delta H$ for a general basis set $(|\alpha\rangle, |\beta\rangle)$. On the other hand, for the basis set that maximizes the norm $\|\Delta H\|$, it is found that the ratio $r$ is negligibly small, as shown in Fig. 2.

Summarizing the above considerations, we have that for weak, strong, and intermediate system-environment coupling strength, maximizing $\|\Delta H\|$ is expected to maximize the $\|\Delta K\|$, and as a result, the properties of PS can be connected with a maximization of $\|\Delta H\|$. Therefore, so long as the impact of $\Delta H$ and $\Delta K$ can be quantitatively captured by their norms $\|\Delta H\|$ and $\|\Delta K\|$, we may consider $\|\Delta H\|$ only. In particular, by maximizing $\|\Delta H\|$, we expect that the two states $|\phi_\alpha(t)\rangle$ and $|\phi_\beta(t)\rangle$ in Eqs. (7) and (8) will evolve most differently, thus yielding an approximate method of predicting and understanding the emergence of PS.

As also stressed in the manuscript, since $\Delta H$ is important in both equations of (7) and (8) $[-\Delta K$ contains $\Delta H$ in Eq. (8)], the contribution of the c-number part of $\Delta H$ (i.e., $H_{\alpha\alpha}^S - H_{\beta\beta}^S$) is nontrivial in determining the PS. Without this c-number term, maximization of $\Delta H$ would incorrectly predict that eigenstates of $H_I$ are the PS regardless of the value of $\varepsilon$. This interesting feature is much different from a pure-dephasing problem. Indeed, in a pure-dephasing problem, there would be no population transitions between $|\phi_\alpha(t)\rangle$ and $|\phi_\beta(t)\rangle$, and hence this c-number term in a pure-dephasing problem would be of no interest: it only induces a phase difference between $|\phi_\beta(t)\rangle$ and $|\phi_\beta(t)\rangle$ and therefore it does not cause the overlap $\langle \phi_\beta(t) | \phi_\alpha(t) \rangle$ to decay.

As two consistency checks, we first return to the first limiting case of $\omega_x \gg \varepsilon$. In this case

$$\Delta H \simeq H_{\alpha\alpha}^S - H_{\beta\beta}^S.$$  (34)

Because eigenstates of $H_S$ correspond to the maximum of $|H_{\alpha\alpha}^S - H_{\beta\beta}^S|$, hence, a maximization of $\|\Delta H\|$, the energy eigenstates of $H_S$ should be the PS. In the second limiting case $\omega_x \ll \varepsilon$, we have

$$\Delta H \simeq \epsilon \left( \langle \sigma_z \alpha \rangle - \langle \sigma_z \beta \rangle \right) \sigma_z^A.$$  (35)

Therefore, the eigenstates of $\sigma_z^A$ and hence the eigenstates of the interaction Hamiltonian $H_I$, can maximize $\|\Delta H\|$, which is again in agreement with the known result that eigenstates of $H_I$ are the PS in this strong coupling case.

[1] S. Goldstein, et al, Phys. Rev. Lett. 96, 050403 (2006).