Quantum dynamical phase transition in a system with many-body interactions

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We introduce a microscopic Hamiltonian model of a two level system with many-body interactions with an environment whose excitation dynamics is fully solved within the Keldysh formalism. If a particle starts in one of the states of the isolated system, the return probability oscillates with the Rabi frequency $\omega_0$. For weak interactions with the environment $1/\tau_{SE} < 2\omega_0$, we find a slower oscillation whose amplitude decays with a rate $1/\tau_0 = 1/(2\tau_{SE})$. However, beyond a finite critical interaction with the environment, $1/\tau_{SE} > 2\omega_0$, the decay rate becomes $1/\tau_0 \propto \omega_0^2 \tau_{SE}$. The oscillation period diverges showing a quantum dynamical phase transition to a Quantum Zeno phase.

Ideal quantum information processing (QIP) involves manipulating a system’s Hamiltonian. In practice, the interactions with an environment perturb the evolution, smoothly degrading the quantum interferences within a “decoherence” rate, $1/\tau_0$. Although one expects $1/\tau_0$ to be proportional to the system-environment (SE) interaction rate $1/\tau_{SE}$, there are conditions where $1/\tau_0$ does not depend on it. This phenomenon was interpreted as the onset of a Lyapunov phase, where the decay rate is the Lyapunov exponent $\lambda$ characterizing the complexity of the classical system. The description of this transition, $1/\tau_0 = \min [1/\tau_{SE}, \lambda]$, requires evaluation of the observables beyond perturbation theory. We will show that a dynamical transition also occurs in a swapping gate: a system that jumps between two equivalent states, $A$ and $B$, when the coupling $V_{AB}$ is turned on. Starting on state $A$, the return probability oscillates with the Rabi frequency $\omega_0 = 2V_{AB}/\hbar$. Since each state interacts with the environment at a rate $1/\tau_{SE}$, weak interactions $(1/\tau_{SE} < 2\omega_0)$ produce a slightly slower oscillation which decays at a rate $1/\tau_0 = 1/(2\tau_{SE})$. However, the swapping frequency is non-analytic on the interaction rate and at a critical strength $1/\tau_{SE} = 2\omega_0$, the oscillation freezes indicating a transition to a new dynamical regime. The initial state now decays to equilibrium at a slow rate $1/\tau_0 \propto \omega_0^2 \tau_{SE}$ which cancels for strong SE interaction. This last regime can be seen as a Quantum Zeno phase, where the dynamics is inhibited by frequent “observations” by the environment. Such quantum freeze can arise as a pure dynamical process governed by strictly unitary evolutions.

We consider a “system” with a single electron occupying one of two coupled states, $A$ or $B$, each interacting with a corresponding electron reservoir (the “environment”). The total system, represented in Fig. 1(a), has the Hamiltonian $\hat{H} = \hat{H}_S + \hat{H}_E + \hat{H}_{SE}$, where the first term is

$$\hat{H}_S = E_A \hat{c}^+_A \hat{c}_A + E_B \hat{c}^+_B \hat{c}_B - V_{AB} (\hat{c}^+_A \hat{c}_B + \hat{c}^+_B \hat{c}_A).$$ (1)

Here, $\hat{c}^+_i$ ($\hat{c}_i$) are the standard fermionic creation (destruction) operators. $E_i$ stands for the energy of the $i$-th local state whose spin index is omitted. $V_{AB}$ yields the natural frequency, $\omega_0 = 2V_{AB}/\hbar$. The environment is

$$\hat{H}_E = \sum_{i=-\infty}^{\infty} \left( E_i |i\rangle \langle i| - \frac{\hbar}{2} \left( \hat{c}^+_i \hat{c}_i + \frac{1}{2} \right) \right) \quad (2)$$

where the sums on negative (positive) index describe a semi-infinite chain to the left (right) acting as a reservoir. $E_{-1} \equiv E_L$ and $E_1 \equiv E_R$ are site energies while $V_{-1} \equiv V_L$ and $V_1 \equiv V_R$ are adjacent site hoppings. The system-environment interaction is modeled with a through-space interaction

$$\hat{H}_{SE} = \sum_{\alpha=\uparrow, \downarrow} \left\{ \sum_{\beta=\uparrow, \downarrow} U^{(dir.)}_{BR} \hat{c}^+_B \beta \hat{c}^{\dagger}_{\beta A} \hat{c}_{\alpha} + \sum_{\beta=\uparrow, \downarrow} U^{(exch.)}_{BR} \hat{c}^+_B \beta \hat{c}^{\dagger}_{\beta A} \hat{c}_{\alpha} + U^{(exch.)}_{AL} \hat{c}^+_A \alpha \hat{c}^{\dagger}_{\alpha B} \hat{c}_{\beta} - U^{(dir.)}_{AL} \hat{c}^+_A \beta \hat{c}^{\dagger}_{\beta B} \hat{c}_{\alpha} \hat{c}_{\alpha} \right\} \quad (3)$$

The first line represents the Coulomb interaction of an electron in state $B$ with an electron in the first site of reservoir to the right. $U^{(dir.)}_{BR}$ is the standard direct integral and $U^{(exch.)}_{AL}$ is the exchange one. Analogously, the second line is the interaction with the reservoir to the left.

A complete norm preserving solution requires the evaluation of the reduced particle and hole density functions $G^R_{ij}(t_2, t_1) = \frac{1}{\hbar} \langle \Psi | \hat{c}_i^+ (t_2) \hat{c}_j (t_1) | \Psi \rangle$ and $G^A_{ij}(t_2, t_1) = -\frac{1}{\hbar} \langle \Psi | \hat{c}_i (t_2) \hat{c}_j^+ (t_1) | \Psi \rangle$ that describe temporal and spatial correlations. Here, the creation and destruction operators are in the Heisenberg representation and $| \Psi \rangle = \hat{c}_{A\beta B}^+ | \Psi_0 \rangle$ is an initial non-equilibrium many-body state built from the non-interacting equilibrium $| \Psi_0 \rangle$. The retarded Green’s function $G^R_{ij}(t_2, t_1) = [G^A_{ij}(t_2, t_1)]^\dagger = \theta (t_2 - t_1) [G_{ij}^R(t_2, t_1) - G_{ij}^R(t_2, t_1)]$ describes the probability amplitude of finding an electron at site $i$ after placing it at site $j$ and letting it evolve under the total Hamiltonian for a time $t_2 - t_1$. By restricting the analysis to $i, j \in \{A, B\}$, $G^R_{ij}(t, t)$ is the single particle $2 \times 2$ density matrix and $G^R_{ij}(t, t_1)$ is an effective evolution operator in this reduced space. In absence of SE interaction, the Green’s function is easily evaluated in its energy representation $G^R_{ij}(\varepsilon) = \int G^R_{ij} (t) \exp[\imath \varepsilon t/\hbar] dt =$
\[ [\varepsilon - H_S]^{-1}. \]

Conversely, the interacting Green’s function defines the reduced effective Hamiltonian and the self-energies \( \Sigma_R(\varepsilon) \), \( H_{\text{eff}}(\varepsilon) \equiv \varepsilon I - \left[ G_R(\varepsilon) \right]^{-1} = H_S + \Sigma_R(\varepsilon) \), where the exact perturbed dynamics is contained in the nonlinear dependence of the self-energies \( \Sigma_R \) on \( \varepsilon \). For infinite reservoirs \( \text{Re} \Sigma_R(\varepsilon) \) represents the “shift” of the system’s eigen-energies \( \varepsilon^{\text{sys}} \) and \( -\text{Im} \Sigma_R(\varepsilon)/\hbar = 1/(2T_{\text{SE}}) \) accounts for their “decay rate” into collective SE eigenstates in agreement with a self-consistent Fermi Golden Rule (FGR), i.e., the evolution with \( H_{\text{eff}} \) is non-unitary.

The complete dynamics will be obtained resorting to the Keldysh formalism. This allows the evaluation of the relevant density-density correlations within a norm conserving scheme:

\[
G^<(t_2, t_1) = \hbar^2 G^R(t_2, t_0) G^<(0, 0) G^A(0, t_1) + \int_0^{t_2} \int_0^{t_1} dt_k dt_l G^R(t_2, t_k) \Sigma^<(t_k, t_l) G^A(t_l, t_1). \tag{4}
\]

The first term stands for the “coherent” evolution while second term contains “incoherent rejections”, described by the injection self-energy, \( \Sigma^< \), that compensates any leak from the coherent evolution. Solving Eq. (4) requires the particle (hole) injection and retarded self-energies, \( \Sigma^<(\cdot)(t_1, t_2) \) and \( \Sigma^R(t_1, t_2) = \theta(t_1, t_2)|\Sigma^>(t_2, t_1) - \Sigma^<(t_2, t_1)| \). For this, we use a perturbative expansion on \( \hat{H}_{\text{SE}} \). The first order gives the standard Hartree-Fock energy corrections which, being real, do not contribute to \( \Sigma^< \). The second order terms, sketched in Fig. 1b), contribute to \( \Sigma^R \), and in the space representation:

\[
\frac{\Sigma^R_{ij}(t_k, t_l)}{\hbar^2} = |U_{is}|^2 G^R_{ss}(t_k, t_l) G^<_{ss}(t_l, t_k) G^A_{ti} G^A_{kt} \delta_{ij}, \tag{5}
\]

where \( (i, s) \in \{(A, L), (B, R)\} \) and hence \( s \) stands for the surface of the site. The net interaction between an electron in the system and one in the reservoir is \( U_{is} = -2U_{(\text{dir})} + U_{(\text{exch})} \), where the direct term contributes with a fermion loop with an extra spin summation. Notice that self-energy diagrams shown in Eq. (1) by describe an electron exciting an electron-hole pair in the environment and later destroying it. The evaluation of these processes requires accounting for the different time scales for the propagation of excitations in the system and reservoirs. We resort to time-energy variables \( t_k = \frac{1}{\hbar} (\varepsilon_k + \delta t_k) \), the physical time, and \( \delta t_k = t_k - t_l \), which characterizes the quantum correlations. The integrand in Eq. (1), when \( t_2 = t_1 \) becomes \( G^R(t_1, (t_1 + \delta t_k)/2) \Sigma^<(\delta t_k, t_l) G^A(t_l - \delta t_k/2, t) \). Since \( \delta t_k \) is related to the energy \( \varepsilon \) through a Fourier transform (FT), in equilibrium,

\[
G^<_{ss}(\varepsilon, t_1) = i 2\pi N_s(\varepsilon) f_s(\varepsilon, t_1), \quad G^>_R(\varepsilon, t_1) = -i 2\pi N_s(\varepsilon) \left[ 1 - f_s(\varepsilon, t_1) \right]. \tag{6}
\]

Here \( N_s(\varepsilon) \) is the local density of states (LDOS) at the surface of the reservoir and \( f_s(\varepsilon, t_1) = \frac{1}{2} \) is the occupation factor in the high temperature limit \( (k_B T \gg V_s) \).

Replacing the LDOS one gets \( G^<_R(\delta t_k, t_1) = \pm i \sqrt{\frac{2J_1(\sqrt{\delta t_k} \delta t_k/2)}{\delta t_k}} \), where \( J_1 \) is the Bessel function of first order. Replacing in Eq. (5),

\[
\frac{\Sigma^R_{ij}(\delta t_k, t_l)}{\hbar^2} = U_{is}^2 \left[ \frac{J_1(\sqrt{4V_s \delta t_k})}{2V_s \delta t_k} \right]^2 G^A_{ti} G^A_{kt} \delta_{ij}. \tag{7}
\]

\[ |J_1[2V_s \delta t_k/\hbar]/(V_s \delta t_k)|^2 \text{ decays in a time scale } h/V_s \text{ which, in the wide-band (WB) limit } V_s \gg V_{AB}, \text{ is much shorter than } h/V_{AB}, \text{ the time scale of } G^<_{ss}(\delta t_k, t_1). \text{ Hence, the main contribution to the integral on } \delta t_k \text{ in Eq. (5) is obtained replacing } G^<_R(\delta t_k, t_1) \text{ by } G^A(0, t_1). \text{ The same consideration holds for } G^R(t_1, (t_1 + \delta t_k)/2) \text{ and } G^A(t_1 - \delta t_k/2, t) \text{ which are replaced by } G^R(t_1, t) \text{ and } G^A(t_1, t). \text{ Then, the dependence on } \delta t_k \text{ enters only through } \Sigma^R_{ij}(\delta t_k, t_1) \text{ yielding }
\]

\[
\Sigma^R_{ij}(t_1) = \int \Sigma^R_{ij}(\delta t_k, t_1) d\delta t_k \tag{8}
\]

\[
= \frac{8}{6\pi} \frac{|U_{is}|^2}{V_s} h G^A_{ti} G^A_{kt} \delta_{ij}. \tag{9}
\]
Hence, in the WB limit, the Keldysh self-energy of Eq. (5) becomes local in space and time and no further structure from higher order terms is admissible. This is represented as a collapse of successive pairs of black dots in Fig. 1b into a single point. The expansion represented in Fig. 1c) and that of Fig. 1d) become exact in this limit.

We assume $E_A = E_B = E_L = E_R = 0$ and the symmetry condition $|U_{AL}|^2 / V_L = |U_{BR}|^2 / V_R$. From Eq. (9) we obtain the decay rates

$$
\frac{1}{\tau_{SE}} = \frac{2 \pi}{\hbar} \text{Im} \Sigma_{ii}^R = \frac{1}{\hbar} \left( \Sigma_{ii}^A - \Sigma_{ii}^R \right) \tag{10}
$$

where $G_{ii}^0 = \left( 4\omega V_{SE}^2 + 1 \right) / \left( 16\omega^2 \tau_{SE} \right)$, with $\alpha = \text{arctan}\left( 1 / (2\omega \tau_{SE}) \right)$ and

$$
\omega = \begin{cases} 2\omega_0 \sqrt{1 - \left( 2\omega_0 \tau_{SE} \right)^{-2}} & \omega_0 > \frac{1}{2\tau_{SE}} \\ 0 & \omega_0 \leq \frac{1}{2\tau_{SE}} \end{cases}, \tag{14}
$$

$$
\eta = \begin{cases} 2\omega_0 \sqrt{(2\omega_0 \tau_{SE})^{-2} - 1} & \omega_0 > \frac{1}{2\tau_{SE}} \\ 0 & \omega_0 \leq \frac{1}{2\tau_{SE}} \end{cases}. \tag{15}
$$

Noticeably, in the first term of Eq. (11) the environment, though giving the exponential decay, does not affect the frequency. Modification of $\omega$ requires the dynamical feedback.

The effect of lateral chains on the two state system can produce observables with non-linear dependences on $H_{SE}$ which could account for a cross over among the limiting dynamical regimes. However, we find a non-analyticity in these functions enabled by the infinite degrees of freedom of the environment (i.e. the thermodynamic limit). Here, they are incorporated through the imaginary part of the self-energy, $\hbar / \tau_{SE}$, i.e. the FGR. Hence, the non-analyticity of $\omega$ and $\tau_{SE}$ on the control parameter $\omega_0 \tau_{SE}$ at the critical value, indicates a switch between two dynamical regimes which we call a Quantum Dynamical Phase Transition.

In the **swapping phase** the observed frequency $\omega$ is finite. According to Eq. (14), if $\omega_0 \tau_{SE} \gg 1$ it coincides with $\omega_0$, indicating a weakly perturbed evolution. As one approaches the critical value $\omega_0 \tau_{SE} = \frac{1}{2}$, $\omega$ decreases vanishing at the critical point. Beyond that value lies the **Zeno phase** where the swapping freezes ($\omega = 0$).

The “decoherence” rate observed from the attenuation of the oscillation is:

$$
\frac{1}{\tau_\phi} = \frac{1}{(2\tau_{SE})} \quad \text{for} \quad \omega_0 \geq \frac{1}{(2\tau_{SE})}. \tag{16}
$$

The dependence of the first term in Eq. (11) on $1/\tau_{SE}$ describes the decay of the initial state into system-environment superpositions. This decay is instantaneously compensated by the “rejection” term which being “in-phase” with the Rabi oscillation ensures $1/\tau_\phi \leq 1/\tau_{SE}$. Beyond the critical value, $\omega_0 \tau_{SE} \leq 1/2$, the decay rate in Eq. (13) **bifurcates into two** damping modes $1/\tau_{SE} \pm \eta$. The slowest, for $\omega_0 \leq \frac{1}{2\tau_{SE}}$, is:

$$
\frac{1}{\tau_\phi} = \frac{1}{2\tau_{SE}} \left[ 1 - \sqrt{1 - \left( 2\omega_0 \tau_{SE} \right)^2} \right] \omega_0 \tau_{SE} \rightarrow \frac{\omega_0^2 \tau_{SE}}{\sqrt{1 - \left( 2\omega_0 \tau_{SE} \right)^2}}. \tag{17}
$$

This manifests the Quantum Zeno Effect: the stronger the interaction with the environment, the longer the survival of the initial state. The critical behavior of the observables $\omega$ and $\tau_{SE}$ is shown in Fig. 2a) and b).

In Fig. 3 different colors label excess or defect in the occupation of state $A$ with respect to equilibrium. The hyperbolic stripes show that the swapping period $T = 2\pi / \omega$ diverges beyond a finite critical value $\omega_0 \tau_{SE} = 1/2$, evidencing the **dynamical phase transition**. Near the critical point $T \simeq (T_c / \sqrt{2}) (1 - T_0 / T_c)^{-1/2}$, where $T_0 = 2\pi \omega_0$

$$
\frac{h}{\tau_{SE}} G_{AA}^<(t, t) = \frac{1}{2} + a_0 \cos \left[ (\omega + \eta) t - \phi \right] e^{-t/(2 \tau_{SE})}, \quad \text{or} \quad \frac{h}{\tau_{SE}} G_{BB}^<(t, t) = \frac{1}{2} + a_0 \cos \left[ (\omega - \eta) t - \phi \right] e^{-t/(2 \tau_{SE})}. \tag{13}
$$
and $T_0^c = 4\pi \tau_{SE}$ is the critical natural period. The critical exponent is $-1/2$. Typical dynamics illustrating both phases are shown at the bottom. Both start with a quadratic decay which is beyond the FGR and results from the phase $\phi$ in Eq. (13).

Related dynamical regimes are predicted for different dissipative two level systems as the spin-boson model initially addressed by Chakravarty and Leggett. While in that model the memory effects are fundamental, our system allows one to reach the strong coupling limit in a case where they are not relevant. Hence, both, $\omega$ and $\tau_{\phi}$, get simple but non-analytic expressions in terms of the control parameter manifesting the critical aspects of the transition to the Zeno phase. This transition has been observed in NMR as an abrupt drop in the frequency and relaxation rate. The present theory also maps to these spin systems.

In summary, a microscopic model for an electron in a two state system coupled to an environment through a many-body interaction shows that by sweeping $\omega_0\tau_{SE}$ below the critical value $1/2$ the oscillatory dynamics freezes. While a crossover to a Zeno regime is expected for strong SE interaction, a non-analytic point separating a finite parametric region of dynamical freeze from a swapping phase defines a quantum dynamical phase transition.

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FIG. 3: (Color online) Contour plot of the particle density function $G_{AA}(t)$ as a function of time and $\omega_0$ in units of $\tau_{SE}$. The vertical line indicates the critical value where the oscillation period diverges. Panels at the bottom show the behavior of $G_{AA}(t)$ for values of $\omega_0\tau_{SE}$ within the Zeno phase (left panel) and the Swapping phase (right panel).