A Quantum Model of Allosteric Signalling as a Non-Markovian Effect

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Allosteric regulation is a central process in biology where binding at one site of a protein has a reversible action at a distance on another functional site. While many questions about the microscopic mechanisms of allostery remain open, many models point to structural (vibrational) dynamics as the carriers of allosteric signals. These degrees of freedom also constitute the primary environments leading to dissipative effects in molecular quantum systems, but inclusion of functional signalling mediated by environments has not been widely studied in open quantum systems. Here we present an allostery-inspired quantum mechanical model where reversible quantum state transitions and environmental energy harvesting are both triggered and controlled by the environmental dynamics induced by a remote two-level system. By employing numerically exact methods based on matrix product state representations of the entire system-environment wave function, we directly demonstrate how the non-perturbative, non-Markovian nature of these dissipative dynamics reproduce a range of features known in biological allostery, potentially opening a path for the exploitation of dissipative signalling in future quantum technologies and nanomaterials.

The theory of open quantum systems (OQS) describes how the unavoidable presence of noisy ‘environmental’ degrees of freedom causes irreversible processes to emerge in quantum dynamics, and underlies our basic understanding of dissipative phenomena such as decoherence, energy relaxation and transport [1, 2]. In many physical cases, system-environment couplings are perturbative, and the action of the environment is to drive weak energy fluctuations of the isolated system states and incoherent transition between them [1, 2]. However, when couplings are strong, environmental ‘back action’ can also change the nature of the system states themselves, profoundly altering the system’s behaviour and responses.

This regime is realized in organic materials, where ‘systems’ such as charges or excitons are strongly coupled to displacements of their molecular structures. Injecting an excitation causes the local structure to relax to a new equilibrium position, but in doing so key system properties such as energy gaps or couplings to other systems can be strongly modified in the new conformation [3, 4]. For typical OQS, these transient ‘reorganization’ dynamics are often irrelevant because they take place on timescales much shorter than the system’s intrinsic dynamics and are typically assumed to act locally, i.e. reorganization dynamics at each sub-system location are uncorrelated [1]. However, for spatially distributed systems in a common medium, such as the chromophores in a protein, it is possible for local reorganization dynamics to propagate and effect dramatic changes at distal locations at later times [5]. This implies that the entire history of the system-environment states becomes relevant, i.e. these dissipative dynamics are manifestly non-Markovian [6], and can only be simulated with state-of-the-art numerical techniques [3, 7, 12].

Despite this challenge, the need to explore such transient out-of-equilibrium phenomena is highlighted by a number of physical examples in which environment-mediated communication and feedback could play an essential functional role, such as the coordination of multiscale, multielectron processes across photosynthetic reaction centres, electron transfer chains and multistage catalysis [13, 16]. Here, we shall take our inspiration from another important biological process: allostery. Allostery refers to the crucial regulation processes in proteins in which the binding of a molecule (ligand) at one site of the protein can have an effect on a distal site (increasing or decreasing the ability to bind). Despite having been conceptualised almost sixty years ago [17, 18], understanding the biophysical mechanisms behind this long-range coupling remains a highly active topic [19, 24]; it is often referred to as “the second secret of life” [25].

In this Letter we introduce a fully quantum mechanical model that describes how the sudden binding of a ‘ligand’ in a bosonic environment can induce spatiotemporal reorganization dynamics capable of reversibly triggering and controlling the quantum dynamics of a remote two-level system (TLS). Exploiting our recent extension of the powerful Time Evolving Density operator with Orthorthonormal Polynomials Algorithm (TEDOPA) method, we demonstrate that the energy of propagating environmental ‘signals’ can be harvested by the TLS to ‘activate’ (populate) metastable excited states. Strikingly, when the TLS is placed closer to the ligand ‘binding’ site, analysis of the system-bath wave functions reveals that static, non-local reorganization can stabilize this activated state, leading to 100% quantum yield and a lifetime that is only limited by the dwell time of the ‘ligand’. The rich phenomenology of this ‘allosteric’ OQS model, together with the forensic capabilities of our new simulation methods, could open up new design concepts for novel, multi-component quantum ‘machines’ and functional materials, as well as provide high-level insights that could be relevant for biological allostery.

A model of quantum allostery. Figure 1 shows schematic representations of allosteric regulation and
is a system projector to the localised state $|i\rangle$. The coupling coefficients between the site $i$ and the mode $k$ are $g^i_k e^{ikr_i}$. The sites $a$ and $b$ have the same coupling coefficients $g^a_k = g^b_k$ and the ratio of the switch coupling coefficients and the site coupling coefficients is $g^S_k/g_k = \sqrt{r}$. The coupling coefficients define the bath spectral density $J(\omega) = \sum_k |g_k|^2 \delta(\omega - \omega_k)$, which we take to have the widely used Ohmic form $J(\omega) = 2\alpha \omega H(\omega_c - \omega)$ where $\alpha$ is the (dimensionless) strength of the system-bath coupling, $H(\omega)$ is the Heaviside function and $\omega_c = c|k_c|$ is the cut-off frequency corresponding to the largest wave-vector $k_c$ of the bath. We use $\omega_c$ as our reference energy scale in all numerical calculations.

Reorganization dynamics. Before proceeding with full quantum simulations of this model, we first build some physical intuition for the action of the reorganization dynamics. Considering the case of a separable system-environment state, the bath part of the interaction Hamiltonian (the last term of Eq. 1) can be treated as an effective external field that creates a space-dependent shift of the system energies given by

$$\Delta E(r_\gamma, t) = \gamma \left\langle \int_R g_k (\hat{a}_ke^{ikr_\gamma} + \text{h.c.}) dk \right\rangle_B .$$

(2)

$\Delta E(r_\gamma, t)$ can be interpreted as work performed by the environment on site $\gamma$ due to its displacement at position $r_\gamma$. For example, if we only consider the switch site ($r = 0$), injecting an excitation here at $t = 0$ would create an energy shift at $r_\gamma$, given by

$$\Delta E(r_\gamma, t) = -\gamma_\gamma 2\lambda \sin(k_cr_\gamma)/k_cr_\gamma + \gamma_\gamma \sum_{\xi = \pm 1} \lambda \sin(k_c(r_\gamma - \xi ct))/k_c(r_\gamma - \xi ct) ,$$

(3)

where $\lambda = \int_0^\infty J(\omega)\omega^{-1} d\omega = 4\alpha \omega_c$ is the bath reorganization energy (see SM [29]). Figure 2 shows the time evolution described by Eq. (3) for $\gamma_\gamma = 1$: the local relaxation of the environment stabilizes the switch excitation on a timescale $\approx \omega_c^{-1}$ (negative energy shift), while two outgoing waves with positive amplitude propagate away from the origin with velocity $c$. These constitute the allosteric signals that will act on the distant TLS in the following sections. Because of the hard cutoff in $J(\omega)$, $\Delta E(r, t)$ is modulated at the wavelength $2\pi/k_c$ due to the Gibbs phenomenon. At long times only the static contribution centered at the position of the excitation remains (first term of Eq. 3), although it has a non-negligible spatial extension ($\approx k_c^{-1}$) and oscillations that will also play an important role in the full quantum allostery dynamics.

Full Quantum dynamics. To study the influence of the transient energy perturbation on the distant TLS, we consider an initial state containing a fully relaxed excitation on site $a$ and an unoccupied switch site. The relaxed initial state of the environment is a coherent state where each mode $k$ has been displaced by an amount

![Schematic representation of an allosteric enzyme. The binding of an effector molecule on the allosteric site can change the configuration of a distal binding site.](image)

FIG. 1. (a) Schematic representation of an allosteric enzyme. The binding of an effector molecule on the allosteric site can change the configuration of a distal binding site. (b) Schematic representation of the system. A two-level system made of sites $a$ and $b$, whose bare energy difference is $E_b - E_a$, is interacting with the same bosonic environment as a so called “switch” site where an excitation is placed at $t = 0$. This excitation will transiently perturb the environment which will have an influence on the energy levels of the two sites.
The dynamics of the state are then simulated with the bath and  \( \hat{\mathcal{D}}_{\delta_k} \) at the speed of sound \( c \).

Transcient system activation. Figure 3 shows the dynamics of the population of site \( b \) for different switch-site distances \( r_a \) and fixed \( k_c R = 4 \) (\( R = r_a - r_b \)). All other parameters are held fixed at zero temperature and with the coupling signs set to \( \varsigma_S = \varsigma_b = -\varsigma_a = 1 \) and \( \kappa a = 1.2 \). The impact of interaction signs on the dynamics is discussed in SM. The choice of opposite signs for sites \( a \) and \( b \) has been made here to enhance the potentiality of a population transfer, but such sign variations occur frequently in common environments associated with protein-bound chromophores \( 31 \). When the perturbation generated by the switch-induced reorganization reaches the system at \( t = r_a/c \), a sudden transfer of population is initiated that can pump over 50% into the higher-energy site \( b \). Once the perturbation has passed, this population decays back to site \( a \) because of downhill energy relaxation. The inset of Fig. 3 shows the evolution of the TLS energy gap as it dramatically closes, as the perturbation raises the energy of site \( a \). This transient near-resonance allows coherent transfer of population through Landau-Zener-type transitions, creating a metastable excited state whose energy could, for example, be directed towards a desired function. The available energy of this state has come directly from the work performed on the system by the reorganization dynamics, and optimizing this would be an interesting area for further work. The timing of this event can be controlled via distance or propagation speed, and we note the highly non-exponential decay of the excited state suggestive of non-Markovian dissipation. Indeed, modification of the spectral function may provide a way to tune the excited state lifetime to match its downstream function. Additionally, unused excitations often have to be deactivated in photosythetic systems to prevent unwanted side reactions, and the dissipation we see corresponds to such deactivation.

Conformational activation. A striking change of behaviour is observed when the TLS is brought closer to the switch site, causing the fate of the excited state to become highly sensitive to the switch-TLS distance. Figure 4 shows the TLS dynamics of the system for smaller \( r_a \), where for \( k_c r_a = k_c R = 5 \), the population is permanently transferred from site \( a \) to site \( b \) with 100% yield. For \( k_c r_a = k_c R = 4,6 \) the yield drops to less than 25%. This stability of population transfer at \( k_c R = 5 \) suggests a last-

\[
\delta_k = -\frac{2w}{\omega_c} e^{-i k r_a}. \text{Throughout, we take} \quad E_b - E_a = 0.5 \omega_c, \quad w = 0.15 \omega_c, \quad \text{and} \quad \alpha = 0.2, \text{so that including the reorganization energy due to the initial relaxation, the total energy gap of the TLS is} \quad E_b - E_a + 2 \lambda = 2.1 \omega_c. \text{This is over ten times larger than the coupling} w, \text{so there is negligible population dynamics in the absence of allosteric signals from the switch (see Fig. 3). At} \quad t = 0^+, \text{we inject an excitation onto the switch site, mimicking the binding of a ligand. The initial joint state for the simulation is thus}
\]

\[
|\psi(t = 0^+)\rangle = |1, 1, 0\rangle_S \otimes \hat{D}(\delta_k)|0\rangle_B \tag{4}
\]

where \( |1, 1, 0\rangle_S \) is the system’s state with an excitation on the switch site, an excitation on site \( a \) and no excitation on site \( b \), \( |0\rangle_B \) is the vacuum state of the bath and \( \hat{D}(\delta_k) \) is a multi-mode displacement operator. The dynamics of the state are then simulated with the numerically exact extension of TEDOPA for correlated environment that was introduced in Ref. \( 30 \) (see SM for details). This delivers the entire joint wave-function \( |\psi(t)\rangle \), and thus allows us visualize and analyse the full quantum dynamics of propagating reorganization including system-environment entanglement and environment-induced dissipation.

The energy shift \( \Delta E(r, t) \) at two times for a Ohmic spectral density with a hard cutoff induced by an excitation at \( r = 0 \) with \( \alpha = 0.1, c = 1 \) and \( k_c = 1 \). The energy shift is composed of a static stabilizing contribution centered on the excitation and two destabilizing contributions, whose amplitudes are half the size, propagating away from the excitation at the speed of sound \( c \).
FIG. 4. Population of site $b$ for different values of $R = r_a$ and $\alpha = 0.2$, $\omega = 0.15\omega_c$ and $\kappa\alpha = 1.2$. For $k_cR = 5$ there is a full population transfer both when the full reorganization dynamics is taken into account and when only the static part of the landscape is considered. In the former case, the population decays back to site $a$ when the switch site is de-excited at $\omega_c t = 200$ (dashed vertical line).

Figure 5(a) shows a heatmap of $\Delta_{ab}E$ for the full population transfer case ($k_cR = 5$). At $t = 0^+$ the switch starts to relax and generate a static negative energy shift at $x = 0$ and two propagating positive energy shifts (only the positive $x$ one is shown) which propagate at the speed of sound. When the right-propagating transient perturbation reaches site $a$, it lifts the energy level of the site and thus initiates population transfer to site $b$. However, once the perturbation passes, the population transfer continues. Fig. 5(b) shows a cross section of the heat maps at the initial and final times and the energy landscape in the hypothetical case where the relaxed switch and relaxed site $a$ coexist. It can be seen that after the switch is fully relaxed, an occupied site $b$ now corresponds to the global ground state of the system, and local environmental dissipation will thus drive the system to this state.

Light can be shed on the distance-dependence of this stabilized transfer by also considering the ‘texture’ of the energy shift induced by the sinc-shaped static part of the energy perturbation generated by the switch. The switch generates a static negative energy shift of large amplitude around the origin and several local minima and maxima that alternate in sign with a wavelength $2\pi/k_c$. The further away from the switch, the lower the amplitude of these extrema (at $k_c x = 10$, 90% of the amplitude has been lost already - see SM [29]). In the $k_cR = 5$ case, site $a$ is close to a maximum of this landscape and is raised in energy. Site $b$ sits on the second maximum, but because it couples to the environment with an negative sign, this static contribution corresponds to a stabilizing negative shift.

For the parameters used in our simulations, these static shifts cause the bare energy of site $b$ to become lower than site $a$, after the switch has relaxed. Although the initial relaxation of the environment around site $a$ still creates a large barrier for population transfer, the static switch potential now renders the population on site $a$ metastable. Thus, the activation of the switch has primed a permanent conformational change in the environment that drives full population transfer. This is directly evidenced in Fig. 4 showing that an excitation initially localized on site $a$ undergoes spontaneous and complete transfer to site $b$, when the environment is initially relaxed in the presence of a populated switch. This observation has a strong implication, namely that this transition should be reversible once the switch is depopulated, as is verified in Fig. 4 for $k_cR = 5$ when we remove the switch excitation at $\omega_c t = 200$. Reversibility of transitions/effects once the effector molecule unbinds is one of the key dynamical features of allosteric regulation, and our model highlights how spatial variations in the non-local energy shift could be exploited for dissipatively ‘locking in’ activated states whose lifetimes are now set by the binding time of a ligand. Finally, in contrast to dynamically activated metastable states, we note that ‘conformationally activated’ states are favoured thermodynamically, i.e. do not harvest energy from the ligand binding directly - the work done by the environment has gone into creating
the driving force for the dissipative population transfer. The deterministic movement of, say, charged excitations to new sites could be used to trigger a wide range of chemical and mechanical processes which could provide catalytic coordination or sensing functions.

**Conclusions.** Our open quantum model of non-Markovian, environmentally mediated signalling exhibits several common features of allosteric regulation, including the distal control of a transition, the reversibility of the transition, the specific spatial arrangement of allosteric and active sites (allosteric pathways), and the mechanical nature of the allosteric signal. Thanks to advanced simulation methods, two distinct classes of allosteric process - dynamical and conformational activation - have been identified, and further work will explore the efficiency of these mechanisms in single-shot and cyclic, i.e. engine, operation. Crucially, while the model is inspired by allosteric 'action-at-a-distance', our quantum model also provides a natural platform to explore strongly non-classical effects in remote signalling, and could naturally be extended to multiparticle systems to explore spatiotemporal entanglement dynamics driven by dissipative processes, i.e. bath reorganization. Indeed, 'quantum' allostery could provide a reversible and non-invasive means of controlling, entangling and probing qubits. Physical 1d platforms such as cold atoms, superconducting qubit chains and ion traps could also be used as quantum simulators for such physics. In the other direction, our model could be refined in multiple ways to describe realistic systems: structured, ab initio spectral densities [32, 33], anharmonic effects [27, 34], and Hamiltonian topologies that account for more complex connectivity between systems and/or environments [3], could all be approached with our present theoretical tools.

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Hamiltonian
\[ \hat{H} = \hat{H}_S + \frac{\hbar \omega}{2}(\hat{X}^2 + \hat{P}^2) + g\hat{S}\hat{X} \]  
\text{(A1)}

where \( \hat{X} \) and \( \hat{P} \) are respectively the dimensionless displacement and dimensionless momentum operators of the harmonic oscillator, \( \hat{S} \) is a diagonal system operator which we will take to be a projector, and \( g \) is the coupling strength between the system and the oscillator. The linear coupling term between the system and the oscillator can be removed by changing \( X \rightarrow X + \hat{A} \), \textit{i.e.} by changing the equilibrium position of the oscillator. Hence the harmonic oscillator’s Hamiltonian becomes
\[ \hat{H}_B = \frac{\hbar \omega}{2}(\hat{X}^2 + \hat{P}^2) \]
\[ = \frac{\hbar \omega}{2}((X - \hat{A})^2 + \hat{P}^2) \]
\[ = \frac{\hbar \omega}{2}(\hat{X}^2 + \hat{A}^2 - 2\hat{X}\hat{A} + \hat{P}^2) \]
\[ \hat{H}_B = \frac{\hbar \omega}{2}(\hat{X}^2 + \hat{P}^2) + \frac{\hbar \omega}{2}(\hat{A}^2 - 2\hat{X}\hat{A}) \] ,  
\text{(A3)}

and the interaction Hamiltonian becomes
\[ \hat{H}_{\text{int}} = g\hat{X}\hat{S} = g\hat{X}\hat{S} - g\hat{A}\hat{S} \].  
\text{(A6)}

We chose \( \hat{A} = \frac{\hbar \omega}{2}\hat{S} \) such that the new linear coupling term \( g\hat{X}\hat{S} \) is canceled out by the linear term \( -\hbar \omega \hat{A} \) from the oscillator’s Hamiltonian.

The Hamiltonian now has the following form
\[ \hat{H} = \hat{H}_S + \frac{\hbar \omega}{2}(\hat{X}^2 + \hat{P}^2) + \frac{\hbar \omega}{2}\hat{A}^2 - g\hat{A}\hat{S} \]  
\text{(A7)}

\[ = \hat{H}_S + \frac{\hbar \omega}{2}(\hat{X}^2 + \hat{P}^2) + \frac{g^2}{2\hbar \omega}\hat{S}^2 - \frac{g^2}{\hbar \omega}\hat{S}^2 \]  
\text{(A8)}

\[ \hat{H} = \hat{H}_S + \frac{\hbar \omega}{2}(\hat{X}^2 + \hat{P}^2) - \frac{g^2}{2\hbar \omega}\hat{S}. \]  
\text{(A9)}

We define the reorganization energy \( \lambda \) \textit{def.} \( \frac{g^2}{2\hbar \omega} \). This reorganization energy comes from a positive contribution from the oscillator’s Hamiltonian and a negative contribution twice as large from the interaction Hamiltonian. Hence, at equilibrium \( \langle \hat{S} \rangle = 0 \), the expectation value of the interaction Hamiltonian is \( \langle \hat{H}_{\text{int}} \rangle = -2\lambda \langle S \rangle \).

**Appendix B: Derivation of the energy shift**

From Eq. \[ \text{B} \] we have an analytic expression for the energy shift
\[ \Delta E(r, t) = \int_{\mathbb{R}} 2g_k \text{Re} \left[ \langle \hat{a}_k \rangle B(t)e^{ikr} \right] dk, \]  
\text{(B1)}

and thanks to Ehrenfest theorem given the Hamiltonian in Eq. \[ \text{I} \] we have
\[ \langle \hat{a}_k \rangle B(t) = \frac{g_k}{\omega_k} \sum_{\alpha} e^{-ikr_{\alpha}} \langle \hat{P}_{\alpha} \rangle e^{-i\omega_k t} - 1 \]
assuming \( \langle \hat{P}_{\alpha} \rangle / (\tau) \approx \text{cst} \).  
\text{(B2)}
Under this assumption, the energy shift can be expressed as
\[ \Delta E(r,t) = \sum_{\gamma} \langle \hat{P}_\gamma \rangle \int_{\mathbb{R}} \frac{2J(k)}{\omega_k} \left[ \cos \left( \omega_k t - k(r-r_\gamma) \right) - \cos \left( k(r-r_\gamma) \right) \right] \, dk . \]
\[ \text{(B3)} \]
This energy shift can be interpreted for each system site as a wave-packet propagating away from the site with an envelope \( \propto J(k)/\omega_k \), plus a static term centered on the site. It can be readily noticed that, because of energy conservation, the energy shift summed over all space at a given time is zero. Trivially, we can see that at \( t = 0 \) the energy shift vanishes. More generally, for a single localised excitation at \( r_\gamma = 0 \) and for any time \( t \)
\[ \int_{\mathbb{R}} \Delta E(r,t) \, dr = \int_{\mathbb{R}} \int_{\mathbb{R}} 2J(\omega_k) \cos \left( \omega_k t - kr \right) - \cos(kr) \, dk , \]
but \( \int_{\mathbb{R}} \cos(\omega_k t - kr) - \cos(kr) \, dk = \delta(k) - \delta(k) = 0 \) as \( \omega_k = 0 \). Hence, conservation of energy is satisfied. The shape of the wave-packet depends on the bath spectral density \( J(k) \). The family of Ohmic spectral densities is labelled by the parameter \( s \) such that \( 0 < s < 1 \) are sub-Ohmic densities, \( s = 1 \) is a Ohmic density and \( s > 1 \) are super-Ohmic densities, for an exponential and a hard cutoff. The spectral density is given by
\[ J(k) = 2\alpha c^2 \frac{|k|^s}{k_c - k} f_{k_c}(k) \]
\[ \text{(B5)} \]
where \( \alpha \) is the strength of the system-bath coupling, \( c \) is the speed of sound, \( k_c \) is the wave-number cut-off of the bath, and \( f_{k_c} \) is a cut-off function equal to \( e^{-|k/k_c|} \) for soft exponential cut-off and to the Heaviside step function \( H(k_c - k) \) for a hard one. For a soft cutoff the energy shift is
\[ \Delta E(r,t) = 4\alpha c k_c \Gamma(s) \left( \frac{-2 \cos \left( \arctan(k_c r)s \right)}{(1 + (k_c r)^2)^{s/2}} \right. \]
\[ \left. + \frac{\cos \left( \arctan(k_c (r - ct))s \right)}{(1 + (k_c (r - ct))^2)^{s/2}} \right) \]
\[ \left. + \frac{\cos \left( \arctan(k_c (r + ct))s \right)}{(1 + (k_c (r + ct))^2)^{s/2}} \right) , \]
\[ \text{(B6)} \]
which reduces in the Ohmic \( (s = 1) \) case to
\[ \Delta E(r,t) = \lambda \left( \frac{-2}{1 + (k_c r)^2} + \frac{1}{1 + (k_c (r - ct))^2} + \frac{1}{1 + (k_c (r + ct))^2} \right) . \]
\[ \text{(B7)} \]
and \( \lambda \) respectively and width \( 1/k_c \). Figure 6 shows the energy shift given by Eq. \( \text{(B7)} \) at different times. The first term is the static negative contribution corresponding to twice the reorganization energy and the two other terms are destabilizing (positive) perturbations propagating away from the site. The stationary state is realized by taking \( t \to \infty \) and corresponds only to the negative static contribution around the position of the site, \( i.e. \) twice the reorganization energy.

For the hard cut-off case, the results are qualitatively the same as in the soft cutoff case but with modulation of the wave packet at the wavelength \( 2\pi/k_c \) due to the Gibbs phenomenon. The energy shift becomes
\[ \Delta E(r,t) = \lambda \left( \frac{-2 \sin(k_c r)}{k_c r} + \frac{\sin(k_c (r - ct))}{k_c (r - ct)} \right. \]
\[ \left. + \frac{\sin(k_c (r + ct))}{k_c (r + ct)} \right) . \]
\[ \text{(B8)} \]

Appendix C: Tensor Networks Simulations, chain mapping

In order to study the population dynamics of the energy barrier, we use a numerically exact method able to handle non-Markovian dynamics that performs the time-evolution of the system and the environment together (enabling us to access not only the system’s dynamics but also the environment’s dynamics). To do so, the non-interacting continuous environment is mapped to two tight-binding 1d-chains with long-range couplings between the system and the environment for the propagating \((k > 0)\) and counter-propagating \((k < 0)\) modes \cite{30,35} using a unitary transformation \( U_{\text{en}}(k) \). The re-
sulting bath Hamiltonian is
\[
\hat{H}_E = \sum_n \omega_n (\hat{c}_n^\dagger \hat{c}_n + \hat{d}_n^\dagger \hat{d}_n) \\
+ t_n (\hat{c}_n^\dagger \delta_{n+1} + \hat{c}_{n+1} \hat{c}_n + \hat{d}_n^\dagger \hat{d}_{n+1} + \hat{d}_{n+1} \hat{d}_n) ,
\]
where \( n \) labels the discrete modes of the new chains, \( \hat{c}_n \) and \( \hat{d}_n \) are the creation operators of these chains with onsite energies \( \omega_n \) and hopping energies \( t_n \), defined by introducing unitary transformations
\[
\hat{a}_{k \geq 0} = \sum_n U_n(k) \hat{c}_n ,
\]
\[
\hat{a}_{-k \geq 0} = \sum_m V_m(k) \hat{d}_m ,
\]
with the matrix elements
\[
U_n(k) = V_n(k) = g_k P_n(k)
\]
where \( \{P_n\}_{n \in \mathbb{N}} \) are orthonormal polynomials with respect to the measure \( \mu(k) = |g_k|^2 \) such that \( P_0(k) = 1 \) and
\[
\int_0^{+k_c} P_n(k) P_m(k) J(k) dk = \delta_{n,m} .
\]

The nature of the polynomials thus depends on the spectral density of the bath. We chose an Ohmic spectral density with a hard cut-off (here at \( k_c \)) \( J(k) = 2\alpha \omega^2 k H(k_c - k) \), where \( \alpha \) is a coupling strength and \( H \) the Heaviside step function. In that case, the \( P_n \) are Jacobi polynomials. Another useful property of these polynomials is that they obey a recurrence relation
\[
P_n(k) = (k - A_{n-1}) P_{n-1}(k) + B_{n-1} P_{n-2}(k) ,
\]
where \( A_n \) is related to the first moment of \( P_n \) and \( B_n \) to the norms of \( P_n \) and \( P_{n-1} \). This recurrence relation can be used to construct the polynomials with the conditions that \( P_0(k) = 1 \) and \( P_{-1}(k) = 0 \), and the recurrence coefficients are used to define the onsite energy \( \omega_n \) and the hopping energy \( t_n \). The interaction Hamiltonian transforms as
\[
\hat{H}_{\text{int}} = \sum_i \gamma_i \hat{P}_i \sum_n \left( \gamma_n(r_i) (\hat{c}_n + \hat{d}_n^\dagger) + \text{h.c.} \right) ,
\]
where \( \gamma_i = \pm 1 \), as defined in Eq. [1] and the new coupling coefficients are
\[
\gamma_n(r_i) = \int_0^{+k_c} g_k e^{i k r_i} U_n(k) dk .
\]

The different system sites couple differently to the chain modes and for a given site the coupling strength across modes is not uniform. A system site at a position \( r \) couples mostly to a specific region of the chain around the mode \( n \sim r \). Since the switch site is situated at the origin, it couples solely to the first mode of each chain.

The joint state of the system and the environment can be described with a Matrix Product State representation and the Hamiltonian can be written in the form of a Matrix Product Operator [20]. We use a tensor network implementation of the time-dependent variational principle to perform the time-evolution [56]. A schematic representation of how the system couples to the chain-mapped environment is shown in Fig. 7.

**FIG. 7.** Schematic representation of the mapping between the system and one of the two chains representing the environment. The switch is only coupled to the first chain mode and sites \( a \) and \( b \) are coupled to every mode with a coupling that is maximal around \( n \sim r_{a/b} \).

**Appendix D: Displaced bath in the chain representation**

Instead of running longer simulations to let the system and the environment reach a steady state in the presence of an excitation at site \( a \), we directly consider a state with a displaced bath. One of the advantage of this is that such a state only takes into account the static part of the reorganization energy. Hence, fewer chain modes are needed because we discard the initial positive perturbations. The complex amplitudes of the displacement \( \delta_k \) of \( k \)-modes for a static excitation since \( t = -\infty \) are
\[
\delta_k = -g_k e^{-ikr_{a/n}} P \left( \frac{1}{\omega_k} \right) ,
\]
where \( P(\cdot) \) is the principal value distribution. For any practical purpose because we use an Ohmic spectral density (which are linear in \( k \)) we can substitute \( g_k P \left( \frac{1}{\omega_k} \right) \) by \( g_k / \omega_k \) if we keep in mind that \( \delta_k = 0 \). The bath displacement operator \( \hat{D} \{\delta_k\} \) can be written in the chain
placements of chain modes are from positive (negative) and \( \hat{\delta} \). The complex displacement amplitude of a chain mode \( r \) is proportional to the Fourier transform of the \( \mathbf{k} \) operator \( \hat{\delta} \). The complex displacement amplitude of a chain mode \( r \) is proportional to the Fourier transform (because \( J \) is proportional to the Fourier transform of the reorganization energy multiplied by the \( n \)th order polynomial defining the chain mapping. For an Ohmic spectral density the displacement is proportional to the Fourier transform of the appropriate polynomial, which might be computed analytically. For an Ohmic spectral density, if \( r_a = 0 \) only the first site of the chain is displaced thanks to the orthogonality of the polynomials. The chain displacement operator \( \hat{D}(\hat{\delta}) \) naturally has a MPO representation with bond dimension 1 as can be seen in Eq. \( D6 \).}

\[
\begin{align*}
\hat{D}(\{\hat{\delta}_k\}) &= \exp \left( \int_{\mathbb{R}^+} (\delta_k \hat{a}_k^\dagger - \delta_k^* \hat{a}_k) dk \right) \\
&= \exp \left( \int_{\mathbb{R}^+} (\delta_k \hat{a}_k^\dagger - \delta_k^* \hat{a}_k) dk \\
&\quad + \int_{\mathbb{R}^+} (\delta_{-k} \hat{a}_{-k}^\dagger - \delta_{-k}^* \hat{a}_{-k}) dk \right) \\
&= \exp \left( \int_{\mathbb{R}^+} (\delta_k \hat{a}_k^\dagger - \delta_k^* \hat{a}_k) dk \\
&\quad \times \exp \left( \int_{\mathbb{R}^+} (\delta_{-k}^* \hat{a}_{-k}^\dagger - \delta_{-k} \hat{a}_{-k}) dk \right) \right) \\
&= \prod_n \exp \left( \int_{\mathbb{R}^+} \delta_k U_n(k) \hat{c}_n^\dagger dk - \text{h.c.} \right) \\
&\quad \times \prod_n \exp \left( \int_{\mathbb{R}^+} \delta_{-k}^* U_n(k) \hat{d}_n^\dagger dk - \text{h.c.} \right) \\
&= \prod_n \exp (\delta_n \hat{c}_n^\dagger - \text{h.c.}) \prod_n \exp (\delta_n^* \hat{d}_n^\dagger - \text{h.c.}) \\
\Rightarrow \hat{D}(\{\delta_k\}) &= \hat{D}(\{\delta_n\}) \\
\end{align*}
\]

where \( \hat{D}(\{\delta_n\}) \) is a displacement operator on the chain and \( \hat{b}_n^\dagger \) (\( \hat{c}_n^\dagger \)) are the chain creation operator originating from positive (negative) \( k \)-vectors. The complex displacements of chain modes are

\[
\delta_n = \int_{\mathbb{R}^+} \delta_k U_n(k) dk \\
= \int_{\mathbb{R}^+} \frac{g_k}{\omega_k} e^{-ikr_a} g_k P_n(k) dk \\
\delta_n(r_a) = -\int_{\mathbb{R}^+} \frac{J(k)}{\omega_k} P_n(k) e^{-ikr_a} dk = -2\pi \mathcal{F} \left[ \frac{J}{\omega} P_n \right] (r_a).
\]

The complex displacement amplitude of a chain mode \( n \) is proportional to the Fourier transform (because \( J(k) \) is non-zero only for positive \( k \)) of the reorganization energy multiplied by the \( n \)th order polynomial defining the chain mapping. For an Ohmic spectral density the displacement is proportional to the Fourier transform of the appropriate polynomial, which might be computed analytically. For an Ohmic spectral density, if \( r_a = 0 \) only the first site of the chain is displaced thanks to the orthogonality of the polynomials. The chain displacement operator \( \hat{D}(\hat{\delta}) \) naturally has a MPO representation with bond dimension 1 as can be seen in Eq. \( D6 \).

**Appendix E: Sign of the interaction Hamiltonian**

To illustrate the influence of the transient energy perturbation on the dynamics of the system, let us consider the following choice of parameters: the gap is \( E_k - E_a = 0.5\omega_c \), the tunneling energy is \( w = 0.15\omega_c \), the separation between the sites is \( k_cR = 10 \), the coupling strength is \( \alpha = 0.4 \), the speed of sound is \( c = 1 \), \( \kappa = 3 \) and \( \varsigma_b = 1 \). With such parameters the initial renormalized energy gap is \( E_b - (E_a - 8\alpha\omega_c) = 3.7\omega_c \gg w \), hence we expect no dynamics for the populations. However, if the switch site is excited at \( t = 0 \), the transient energy perturbation should affect the energy of site \( a \) and site \( b \) respectively around the times \( t = R/c \) and \( t = 2R/c \), and could induce some dynamics because the renormalized gap is reduced for a short amount of time. The dynamics of the gap between the two sites will also depend on the sign of \( \varsigma_b \). A positive sign would mean that the perturbation increases the gap and a negative sign reduces the gap. Figure 8 shows the evolution of the population of site \( b \) for both values of \( \varsigma_b \). In both cases the dynamics is radically altered as the population grows instead of staying at zero. When \( \varsigma_b = -1 \), two steps are visible and can be clearly associated with the transient energy perturbation. In the opposite case, the population stays constant after the first step. Indeed, the gap becoming larger when the perturbation reaches site \( b \) prevents further population transfer. With this first example we can already see that non-trivial population transfer can be induced by the environment.

**Appendix F: Switch displacement trajectories**

Figure 9 shows a heatmap of the energy shift generated by the switch for \( \kappa \alpha = 1.2 \).
FIG. 9. Map of the energy perturbation generated by the switch. Transient perturbation of amplitude $\lambda S = 4\kappa\alpha\omega_c$ are sent away in space, and a static contribution of amplitude $-2\lambda S$ is centered around the switch. The vertical lines mark the position of site $a$ at $x = 5$ and site $b$ at $x = 10$.

**Appendix G: Influence of the coupling strength**

The amount of population transferred can be controlled via the coupling strength between the system and the bath as it depends on the renormalized gap between the two sites. The higher the coupling to the bath, the larger the reorganization energy. Thus at a fixed amplitude of the energy perturbation – holding $\kappa\alpha$ constant –, increasing the coupling strength between the system and the bath leads to a decrease of the transferred population as the barrier to be crossed becomes higher. For larger values of $\alpha$, the occupied site $b$ states becomes even more favoured thermodynamically but, because of the increase of the initial gap, the transfer of population slows down. Figure 10 shows how the population of site $b$ is impacted by $\alpha$. 
FIG. 10. Population of site $b$ for different coupling strength $\alpha$ with $R = 5$, $w = 0.15$, $\omega_c = 1$, $c = 1$ and $k\alpha = 1.2$. The dashed vertical lines indicate the time at which the perturbation reaches the sites $a$ and $b$. The horizontal dotted line shows half population. Long lasting partial and total population transfer are initiated by the effect of the switch.