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Topological transition of a non-Markovian dissipative quantum walk

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We extend non-Hermitian topological quantum walks on a Su-Schrieffer-Heeger (SSH) lattice [Phys. Rev. Lett. 102, 065703 (2009)] to the case of non-Markovian evolution. This non-Markovian model is established by coupling each unit cell in the SSH lattice to a reservoir formed by a quasicontinuum of levels. We find a topological transition in this model even in the case of non-Markovian evolution where the walker may visit the reservoir and return to the SSH lattice at a later time. The existence of a topological transition does, however, depend on the low-frequency properties of the reservoir, characterized by a spectral density $J(\epsilon) \propto |\epsilon|^\alpha$. In particular, we find a robust topological transition for a sub-Ohmic ($\alpha < 1$) and Ohmic ($\alpha = 1$) reservoir, but no topological transition for a super-Ohmic ($\alpha > 1$) reservoir. This behavior is directly related to the well-known localization transition for the spin-boson model. We confirm the presence of non-Markovian dynamics by explicitly evaluating a measure of Markovianity for this model.

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I. INTRODUCTION

Quantum walks represent the quantum version of classical random walks [1–3] where a particle, the “walker,” moves on a lattice, evolving into a superposition of states. The walker may possess internal degrees of freedom in addition to the spatial degree of freedom. Translation of the particle may then depend on its internal state. Quantum walks can be used as a platform for universal quantum computation [4] or to study topological phases [5–7]. For quantum walks, a topological phase can be inferred from the observation of boundary states [8,9], from bulk observables, such as the mean chiral displacement [10,11], or directly from a winding number [12]. Quantum walks have been extended using the language of open quantum systems [13,14] with applications to photosynthetic energy transfer [15,16] and environment-assisted transport [17]. Quantum walks have also been extended to account for non-Markovian evolution [18,19], describing information backflow from an environment.

In non-Hermitian quantum walks, the walker can escape from the lattice with a decay rate showing up as a non-Hermitian term in the Hamiltonian [12,20,21]. Early work on non-Hermitian quantum walks extended the Su-Schrieffer-Heeger (SSH) model in this way by including an on-site imaginary energy and introduced a bias potential on sublattice sites. The SSH model consists of a one-dimensional chain with dimerized (alternating) tunnel coupling between sites, one for intracell hopping and another for intercell hopping. In the non-Hermitian topological quantum walk based on the extended SSH lattice [12], the average displacement achieved by the walker before leaving the lattice is a topological invariant, given by a winding number. This winding number changes only at a critical ratio of the intercell-to-intracell coupling and is otherwise unaffected by details of the system [12,22]. In $k$ space, the tunnel coupling becomes a complex number described by a magnitude and a phase. The winding number represents the number of times this phase winds as $k$ traverses the Brillouin zone. This winding number is important, in general, to classify the topological phases of non-Hermitian one-dimensional systems [23].

In this paper, we derive the condition for a topological transition in an alternative extended version of the SSH model where, in each unit cell, a lattice site is coupled to a reservoir formed by a quasicontinuum of levels. We study the resulting dynamics of the walker in this extended model without performing the Markov approximation. Recently, other extensions of the SSH model that include additional sites in each unit cell have been studied, and the chiral displacement has been analyzed in these models [11]. Here, we go beyond this analysis allowing for a general structure of the reservoir having a quasicontinuous bath spectral density, which reduces to the model of Ref. [12] in a well-defined Markovian limit. In fact, we find (for this generalized model) that the presence of a topological transition is determined through the low-frequency properties of the reservoir, characterized by the spectral density $J(\epsilon) \propto |\epsilon|^\alpha$ with exponent $\alpha$. In particular, we find a robust topological transition for a sub-Ohmic ($\alpha < 1$) and an Ohmic ($\alpha = 1$) reservoir, but no topological transition for a super-Ohmic ($\alpha > 1$) reservoir. This behavior is directly related to the well-known localization transition in the spin-boson model [24].

Remarkably, even in the case of non-Markovian evolution where the walker may visit the reservoir and return, we find a robust topological phase transition in terms of the time-averaged mean displacement, which again can be written in terms of a winding number. We confirm the presence of non-Markovian dynamics in this model directly through Breuer’s measure of Markovianity [25]. This problem is analogous to
the Weisskopf-Wigner model for the spontaneous decay of a two-level atom coupled with a continuum of radiation modes [26]. Thus, it may be possible to probe these results in experiments on stimulated Raman adiabatic passage (STIRAP) [27] or in cold-atom systems with a controllable spectral density [28].

This paper is organized as follows: In Sec. II, we present the lattice and the Hamiltonian. In Sec. III, we derive the conditions under which the topological invariant of interest, the long-time time-averaged displacement, can be obtained in terms of the winding number. In Sec. IV, the problem is mapped to the Weisskopf-Wigner model as a special case of the spin-boson model. This will prove to be useful once the low-frequency properties of the environment are described in terms of a spectral density $J(\epsilon) \propto |\epsilon|^\nu$, a problem already encountered for the spin-boson model [24]. In Sec. V, we lay down the quantum-dynamical formalism used to calculate the topological invariant found in Sec. II. In Sec. VI, we study the non-Markovian properties of the system using a measure derived in Ref. [25]. In Sec. VII, we draw conclusions and discuss possible experimental realizations of the model.

II. QUANTUM-WALK HAMILTONIAN

The quantum walk that we study describes hopping of a quantum particle on a translationally invariant one-dimensional chain with unit cells labeled by an integer $m$ and a staggered (dimerized) coupling between $A$ and $B$ sublattice sites [see Fig. 1(a)]. The dense set of levels $C$ explicitly models a reservoir that the walker can enter and exit via state $B$ as it moves through the lattice. We therefore label the state of the walker by $m$ and $j \in \{A, B, j\}$, where $j$ indexes the levels within $C$. This model generalizes the non-Hermitian quantum walk studied in Ref. [12] where the walker could only leave the lattice from sites $B$ without the possibility to return.

In direct analogy with the non-Hermitian quantum walk, for the present model, we take the escape probability to be the probability to leave sublattice $A$, i.e., the probability to be either on a $B$ site or in one of the levels $C$. In the rest of this paper, we will group $B$ sites and $C$ levels in each unit cell into a common reservoir. The observable of interest, the average displacement, is the average distance (number of unit cells) traveled by the walker before leaving sublattice $A$ (reaching a reservoir, i.e., sublattice sites $B$ or $C$). This leads to the central question of this paper: Is the topological transition found in Ref. [12] still present when we allow for non-Markovian dynamics of the walker?

We express the quantum-walk Hamiltonian as a sum of terms $H = \hat{H}_A + \hat{H}_A + V$ with

$$\hat{H}_A = \sum_{m=\infty}^{\infty} \epsilon_A[A, m]|A, m\rangle \langle A, m|,$$

$$\hat{H}_A = \sum_{m=\infty}^{\infty} (\epsilon_A + \omega)|B, m\rangle \langle B, m| + \sum_{j \in C} \epsilon_j|j, m\rangle \langle j, m| + \sum_{j \in C} (g_j|j, m\rangle \langle B, m| + \text{H.c.}),$$

$$V = \sum_{m=\infty}^{\infty} \langle v|A, m\rangle \langle B, m| + v'|A, m\rangle \langle B, m + 1| + \text{H.c.}.$$
with
\[ H_A(k) = \varepsilon_A |A, k\rangle \langle A, k|, \]
\[ H_A(k) = (\varepsilon_A + \omega) |B, k\rangle \langle B, k| + \sum_{j \in C} \varepsilon_j |j, k\rangle \langle j, k| \]
\[ + \sum_{j \in C} (g_j |j, k\rangle \langle B, k| + H.c.), \]
\[ V(k) = |v(k)\rangle \langle v(k)| \langle A, k| \langle B, k| + H.c.). \]

Here, the angle \( \phi(k) \) is the argument of the complex hopping amplitude \( v(k) = v + \nu' e^{i\kappa} \),
\[ \phi(k) = \text{arg}[v(k)] = \text{arg}[v(1 + u e^{i\kappa})], \quad u = \frac{\nu'}{v}. \]
The parameter \( u \), the ratio of intercell to intracell hopping amplitudes, controls the topological transition that was investigated in the related non-Hermitian quantum walk studied in Ref. [12].

III. QUANTUM-WALK EVOLUTION

We now analyze the evolution of a quantum walker initialized in state \( A \) within unit cell \( m = 0 \),
\[ \psi_{lm}(0) = |l, m\rangle \langle \psi(0)| = \delta_{l, A} \delta_{m, 0}. \]

Our goal is to evaluate the average number of unit cells traversed by the walker before leaving sublattice \( A \) in the long-time limit under evolution governed by the Hamiltonian \( H \) defined in Sec. II. To evaluate this quantity, we first define a set of probabilities \( \{\rho_{Am}(t)\} \), where
\[ \rho_{Am}(t) = \sum_{l \notin A} |\psi_{lm}(t)|^2 \]
gives the probability that the walker resides in the reservoir of unit cell \( m \) at time \( t \).

In terms of the probabilities in Eq. (9), the average displacement at time \( t \) is given by
\[ \langle m(t) \rangle = \sum_m m \rho_{Am}(t). \]

In \( k \) space, Eq. (10) can be rewritten using the probability density \( \rho_A(k, t) \) at quasimomentum \( k \) and at time \( t \) (see Appendix A),
\[ \langle m(t) \rangle = \int dk \frac{\partial \phi(k)}{\partial k} \rho_A(k, t), \]
where
\[ \rho_A(k, t) = \sum_{l \notin A} |\langle l, k|\psi(t)\rangle|^2 = \sum_{l \notin A} |\psi_l(t)|^2. \]

Non-Markovian (history-dependent) dynamics can give rise to nondecaying persistent oscillations of the probability density \( \rho_A(k, t) \) [see, e.g., Fig. 2(b) below]. Hence, in general, the long-time limit of Eq. (11) is not necessarily well defined. As an alternative, we characterize the average displacement before leaving sublattice \( A \) by the long-time time-averaged value \( \langle m \rangle \),
\[ \langle m \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \langle m(t) \rangle = \int dk \frac{\partial \phi(k)}{\partial k} \rho_A(k), \]
where the long-time-averaged probability to find the walker in the reservoir is given by
\[ \rho_A(k) = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \rho_A(k, t). \]

The spatially localized initial state [Eq. (8)] corresponds to a uniform distribution in \( k \) space,
\[ \rho_A(k, 0) = |\psi_A(k, 0)|^2 = \frac{1}{2\pi} \quad \forall k, \]
which, together with the conservation of \( k \), implies the normalization condition \( \rho_A(k) + \rho_A(k) = 1/(2\pi) \). The probability density \( \rho_A(k) = 1/(2\pi) - \rho_A(k) \) controls the behavior of \( \langle m \rangle \), the central quantity of interest in this paper [see Eq. (13)]:

Fig. 2. Evolution of the average displacement \( \langle m(t) \rangle \) (blue dashed lines) and the probability \( 2\pi \rho_A(k = 0, t) \) (green solid lines) as a function of time. For simplicity, we take \( v > 0 \) and set the dimensionless quantities \( J_A v^{\nu+1} = 0.01, \Delta/v = 5, u = v'/v = 2.0 \). Here, \( \alpha = 0 \) in (a) and \( \alpha = 2 \) in (b). For \( \alpha < 1 \), the walker decays completely into the reservoir, and the average displacement approaches \( \langle m(t) \rangle \rightarrow 0 \) at long times for \( u = v'/v > 1 \). For \( \alpha > 1 \), the walker never decays completely into the reservoir, and \( \rho_A(k = 0, t) \) oscillates about the long-time average value [black dotted line in (b)] given by Eq. (34).
If $\rho_k(t) = 1/(2\pi)$ [i.e., $\rho_k(t) = 0$ for all $k$], the walker ends up in the reservoir with certainty in the long-time limit, and the average displacement is simply given by a winding number,

$$\langle m \rangle = \frac{\Delta \phi}{2\pi} = \oint dk \frac{\partial \phi(k)}{2\pi \partial k} = \theta(|u| - 1), \quad (16)$$

where $\theta(x)$ is the Heaviside step function. Equation (16) results in a topological phase function from $\langle m \rangle = 0$ to $\langle m \rangle = 1$ at a critical value of $|u| = |v'/v| = 1$. This was also the result found for the Markovian quantum walk studied in Ref. [12]. Our goal is now to find the conditions under which the walker decays completely into the reservoir in the long-time limit.

### IV. MAPPING TO THE WEISSKOPF-WIGNER MODEL

In this section, we map the lattice model to the Weisskopf-Wigner model for a two-level atom coupled to radiation modes. This mapping to the Weisskopf-Wigner model gives further insight into the nature of the problem, simplifies the modes. This mapping to the Weisskopf-Wigner model gives the Wigner model for a two-level atom coupled to radiation.

For $\{0\}$, we associate the state where the walker is in reservoir state $|0\rangle$ is in the excited state and no photons are in the continuum. Figure 1(b) depicts the level structure described by Eq. (19).

For each fixed wave-number $k$, the quantum walk problem [as described by Eq. (19)] can be directly mapped to the Weisskopf-Wigner model [26] for an atom decaying into a continuum of radiation modes (the environment): Having the walker on site $A$ can be associated with a state where the atom is in the excited state and no photons are in the continuum. We associate the state where the walker is in reservoir state $j \in C$ with an atomic ground state and one photon in the environment in mode $j$. The formal mapping between these two descriptions is as follows:

Quantum walk $\leftrightarrow$ Weisskopf-Wigner model,

$$|A, k\rangle \leftrightarrow |A, k\rangle \otimes |0\rangle, \quad (20)$$

$$|j, k\rangle \leftrightarrow |C, k\rangle \otimes |j\rangle, \quad (21)$$

where $|A, k\rangle = |e\rangle$ labels the atom in the excited state, $|0\rangle$ labels the vacuum state of the environment with 0 photons, $|C, k\rangle = |g\rangle$ labels the atomic ground state, and $|j\rangle$ labels the state of the environment with one photon in state $j$. The quantum walk maps onto a family of Weisskopf-Wigner models, one for each value of $k$ with a $k$-dependent coupling $\eta_j(k)$.

Relative to the quantum walk, there are additional states introduced in the Weisskopf-Wigner model. These states contain different numbers of excitations: state $|C, k\rangle \otimes |j\rangle$ with no excitations in the atom or environment, and states $|A, k\rangle \otimes |j'\rangle$ and $|C, k\rangle \otimes |j'\rangle$, where $j'$ may denote a state with an arbitrary number of excitations in the environment. The initial state in Eq. (8) has only one excitation (i.e., the atom is excited, and the reservoir is in its vacuum state). Since the Hamiltonian preserves the total number of excitations, the additional states with different numbers of excitations will never become occupied. Therefore, all time-dependent observables evaluated in the Weisskopf-Wigner model with the appropriate initial condition will map identically to observables in the non-Markovian quantum walk. The mapping to an enlarged Hilbert space (associated with the Weisskopf-Wigner model) will, however, be useful when evaluating a test of non-Markovianity in Sec. VI.

Equation (13) shows that the topological transition (for which the average displacement $\langle m \rangle$ is quantized) is realized if the walker decays completely into the reservoir, leading to $\rho_k(t) = 1/(2\pi)$. The mapping to the Weisskopf-Wigner model allows us to reformulate the question of a topological transition in terms of a question about a decaying atom. In particular, we ask the question: Under which conditions does the atom decay to its ground state in the long-time limit? This question has been addressed previously in the context of the spin-boson model [24,29]. The spin-boson model is a general description of a two-level system (here, $|A, k\rangle$, $|C, k\rangle$) coupled to a bosonic bath. Depending on the spectral density of the bath, the dynamics of the two-level system initialized in $|A, k\rangle$ can either show damped coherent oscillations between states $|A, k\rangle$ and $|C, k\rangle$ with a bounded degree of decay (occupying both $|A, k\rangle$ and $|C, k\rangle$ with a finite probability in the long-time limit), or decay to zero, occupying only $|C, k\rangle$ at long times. In the quantum walk, this second scenario corresponds to
the walker leaving sublattice $A$, $\rho_A(k) = 0$ for $\rho_A(k) = 1/2\pi$, which, in turn, leads to the desired topological transition. The topological transition can, therefore, be controlled through the reservoir spectral density as in the case of the spin-boson model [24,29].

Note that the above analysis of the Weisskopf-Wigner model assumes an initial zero-temperature reservoir containing no excitations. At finite temperatures, the reservoir would have a thermal population of photons. This would lead to absorption that would, in general, lead to a nonvanishing temperature-dependent stationary excited-state probability for the atom. On the other hand, the original formulation of the problem describes a single particle hopping on a lattice, which is out of equilibrium and, thus, the notion of temperature does not necessarily apply.

**V. LONG-TIME DYNAMICS OF THE WALKER**

The average displacement [Eq. (13)] is given in terms of the long-time time-averaged probability density $\rho_A(k)$ [Eq. (14)], which, in turn, can be found from the complementary probability to remain in sublattice $A$; $\rho_A(k) = 1/2\pi - \rho_A(k)$. The Nakajima-Zwanzig generalized master equation [30,31] can be used to find the time-dependent probability density $\rho_A(k, t)$ without resorting to a Markov approximation. In this section, we work in the language of the Weisskopf-Wigner model where the state of the walker (atom) is described by the manifold $\{|A, k\rangle, \{C, k\rangle\}$ and the state of the environment is independently described by $\{|0\rangle, |j\rangle\}$. After tracing out the reservoir (environment) degrees of freedom, the Nakajima-Zwanzig generalized master equation gives an equation of motion for the state of the walker (atom) alone.

The generalized master equation for $\rho_A(k, t)$ in the Born approximation (second order in $\vec{h}_i$) assumes the simple form (see Appendix C),

$$\dot{\rho}_A(k, t) = -i \int_0^t dt' \Sigma_A(k, t-t')\rho_A(k, t'),$$  

(23)

where the self-energy $\Sigma_A(k, t)$ is given by

$$\Sigma_A(k, t) = -2i \sum_j |\vec{h}_j(k)|^2 \cos(\epsilon_j t).$$  

(24)

We take the Laplace transform of Eq. (23) $f(s) = \int_0^\infty dt e^{-st} f(t)$ for any function $f$ and find

$$\tilde{\rho}_A(k, s) = \frac{\rho_A(k, 0)}{s + i\Sigma_A(k, s)} = \frac{1}{2\pi} \frac{1}{s+i\Sigma_A(k, s)},$$  

(25)

with

$$\Sigma_A(k, s) = -2i \int dt J(k, e) \frac{s}{s^2 + \epsilon^2}.$$  

(26)

We introduce the spectral density $J(k, \epsilon)$ as

$$J(k, \epsilon) \equiv \sum_j |\vec{h}_j(k)|^2 \delta(\epsilon - \epsilon_j).$$  

(27)

To find $\rho_A(k, t)$, we invert Eq. (25) using the Bromwich inversion integral,

$$\rho_A(k, t) = \frac{1}{2\pi i} \int_C ds e^{st} \frac{\rho_A(k, 0)}{s+i\Sigma_A(k, s)}.$$  

(28)

defined on the contour $C$ running along the vertical line $Re(s) = \gamma > 0$ such that all singularities lie to the left of $C$. The different possible nonanalytic features of $\rho_A(k, t)$ give rise to different forms of decay in real time: Exponential decay arises from isolated poles at $s = sj$, with $Re(sj) < 0$, long-time power-law tails arise from branch-cut integrals, and persistent oscillations arise from poles at $s = sj$, with $Re(sj) = 0$.

In terms of the Laplace transform, the long-time average of $\rho_A(k, t)$ $\rho_A(k, 1/2\pi - \rho_A(k)$ with $\rho_A(k)$ defined in Eq. (14) is simply given by the residue at $s = 0$,

$$\rho_A(k) = \lim_{s \to 0} s\tilde{\rho}_A(k, s) = \frac{1}{2\pi} \frac{1}{1+i\Sigma_A(k)},$$  

(29)

$$\Sigma_A(k) = \lim_{s \to 0} \frac{\tilde{\Sigma}_A(s, k)}{s}.$$  

(30)

Contributions from all other terms either decay or oscillate about zero, vanishing under the average given in Eq. (14).

In the continuum limit, the sum in Eq. (27) is converted to an integral, and $J(k, \epsilon)$ becomes a quasicontinuous function. We distinguish two cases. When $J(k, \epsilon = \epsilon_A) \neq 0$, $\Sigma_A(k) \to \infty$, and $\rho_A(k) \to 0$ [see Eq. (29)], i.e., the walker decays completely into the reservoir. The situation is more complicated when $J(k, \epsilon = \epsilon_A) = 0$. In this case, we assume the low-frequency spectral density is described by a power-law behavior,

$$J(k, \epsilon) = J_0 |v(k)|^2 \epsilon^\alpha, \quad 0 \leq \alpha \leq \Delta, \quad (31)$$

with spectral exponent $\alpha \geq 0$ and $J_0$ is a dimensionful prefactor. We have introduced a sharp cutoff in the spectral density for frequencies higher than a bandwidth $\Delta > 0$. The spectral exponent characterizes the type of reservoir: sub-Ohmic for $\alpha < 1$, Ohmic for $\alpha = 1$, and super-Ohmic for $\alpha > 1$.

We insert Eq. (31) into Eq. (26) and integrate over the finite bandwidth, giving

$$\tilde{\Sigma}_A(k, s) = -i \Omega_\alpha^+ \frac{\Omega_\alpha^-}{s} 2F_1\left(\frac{1}{2} \alpha + 1, \frac{1}{2} \alpha + 3, \frac{\Delta^2}{s^2}\right),$$  

(32)

Finally, we calculate $\rho_A(k)$ by inserting Eq. (32) into Eq. (29),

$$\rho_A(k) = \begin{cases} 0, & 0 \leq \alpha \leq 1, \\ \frac{1}{\pi^2 \Gamma(\alpha)} \alpha > 1. \end{cases}$$  

(34)

The result in Eq. (32) and the subsequent limit in Eq. (34) also arise in the problem of Brownian motion for a quantum particle (Eqs. (11.1)–(11.3) in Ref. [32]).

We have found that the walker decays into the continuum if $0 \leq \alpha \leq 1$. Otherwise, there is a residual probability to find the walker on sites $A$ in the long-time limit, given by Eq. (34). The dissipative dynamics of the spin-boson model has been studied for the spectral density in Eq. (31) [24,29]. At zero temperature, for $\alpha \leq 1$ (for an Ohmic or a sub-Ohmic spectral density) the spin is localized (the walker ends up in the reservoir), whereas for $\alpha > 1$ (for a super-Ohmic spectral density), the system undergoes persistent coherent oscillations between the two spin states (the walker moves back and forth...
is not protected for $\alpha > 1$, in which case the average displacement is not quantized. In Fig. 3(b), we show $\langle m \rangle$ along two vertical cuts of Fig. 3(a) (corresponding to $\alpha = 0.5$ and $\alpha = 1.5$). This phase diagram extends the result obtained for a Markovian quantum walk in Ref. [12]. The extreme Markovian limit in our model corresponds to an infinite-bandwidth flat spectral density ($\alpha = 0$, $\Delta \to \infty$). In this limit, we recover the results of Ref. [12], which is to be expected since the two models are equivalent in the Markovian limit. In contrast with Ref. [12], here, no Markov approximation was performed, and we have solved the problem for a generalized spectral function characterized by a general non-negative low-energy spectral exponent $\alpha$.

VI. NON-MARKOVIAN NATURE OF THE QUANTUM WALK

In this section, we check explicitly that the dynamics of the system is non-Markovian using a method similar to that described in Ref. [25], which we summarize here.

The Breuer measure of non-Markovianity [25] for quantum evolution is defined as

$$\mathcal{N} = \max_{\rho_{1,2}(0)} \int_{\tau > 0} dt \, \sigma[t; \rho_{1,2}(0)].$$  \hspace{1cm} (35)

Here, $\sigma[t; \rho_{1,2}(0)]$ is the rate of change in the trace distance between two density matrices $\rho_1(t)$ and $\rho_2(t)$, assumed to evolve according to the same dynamical map,

$$\sigma[t; \rho_{1,2}(0)] = \frac{d}{dt} \mathcal{D}[\rho_1(t), \rho_2(t)],$$  \hspace{1cm} (36)

where $\rho_1(0)$ and $\rho_2(0)$ are the initial conditions from which $\rho_1(t)$ and $\rho_2(t)$ evolved. The trace distance is defined as

$$\mathcal{D}[\rho_1, \rho_2] = \frac{1}{2} \text{Tr}|\rho_1 - \rho_2|,$$  \hspace{1cm} (37)

where $|A| = \sqrt{A^\dagger A}$. The integral in Eq. (35) is restricted to $\sigma > 0$, and the result is maximized over all possible initial conditions $\rho_{1,2}(0)$.

The trace distance is a monotonic decreasing function of time when the evolution of the density matrices is given by a completely positive and trace preserving map. This is the case, for example, for a Markovian process. In these cases, $\sigma$ is never positive,

$$\sigma[t; \rho_{1,2}(0)] \leq 0,$$  \hspace{1cm} (38)

and $\mathcal{N} = 0$. Thus, to prove that the evolution is non-Markovian, it is sufficient to show that $\sigma$ becomes positive at certain times and for some initial states $\rho_{1,2}(0)$: $\sigma[t; \rho_{1,2}(0)] > 0$, yielding $\mathcal{N} > 0$.

We work with the reduced density matrix obtained by marginalizing over all wave-vectors $k$,

$$\rho_{1,2}(t) = \sum_{l,l'} |l\rangle \langle l'| \int dk \, \text{Tr}_E[\langle l, k| \rho_{1,2}(t)|l', k\rangle],$$  \hspace{1cm} (39)

where $\text{Tr}_E$ is the partial trace over the environment degrees of freedom describing the photon state for the Weisskopf-Wigner problem: $\text{Tr}_E[O] \equiv \langle 0|O|0\rangle + \sum_{j} \langle j|O|j\rangle$ for any operator $O$. Here, $l, l' \in \{A, C\}$ label quantum numbers for a fictitious two-dimensional auxiliary space that makes it convenient to
calculate the total probability $p_A(t)$ for the walker to be found in sublattice $A$ at time $t$.

State $\rho_{1,2}(t)$ in Eq. (39) is the full density matrix in the enlarged Hilbert space of the Weisskopf-Wigner problem at time $t$, conditioned on the initial states,

$$\rho_1(0) = |A, m = 0 \rangle \langle A, m = 0| \otimes |0 \rangle \langle 0|,$$

$$\rho_2(0) = |C, m = 0 \rangle \langle C, m = 0| \otimes |0 \rangle \langle 0|.$$

The initial condition $\rho_1(0)$ describes a uniform coherent superposition of Weisskopf-Wigner problems with different $k$’s corresponding to an atomic excited state $A$ with no photons in the environment ($|0\rangle$). This is equivalent to having the walker initialized to sublattice $A$, localized at lattice site $m = 0$ [Eq. (8)]. We compare evolution with this initial condition to the trivial evolution found with the initial condition $\rho_2(0)$. State $\rho_2(0)$ corresponds, instead, to having the atom in the ground state and no photons in the environment in the Weisskopf-Wigner model. This is equivalent to having no walker. Since $\rho_1(0)$ and $\rho_2(0)$ in Eqs. (40) and (41) describe orthogonal pure states, this choice of two initial states maximizes the trace distance Eq. (37) at $t = 0$.

The time evolution of $\rho_2(t)$ is trivial $\rho_2(t) = \rho_2(0)$ since the initial condition describes a state with no excitations (no walker). For the initial condition $\rho_1(0)$, we find the future evolution of $\rho_1(t)$ is given by (see Appendix C)

$$\rho_1(t) = \rho_A(t)|A\rangle \langle A| + [1 - \rho_A(t)]|C\rangle \langle C|,$$

$$p_A(t) = \int dk \rho_A(k, t),$$

where the total probability for the walker to be on sublattice site $A$, $p_A(t)$, is simply found by integrating the probability density $\rho_A(k, t)$ over $k$.

From Eq. (37), we find that the trace distance can be expressed directly in terms of $p_A(t)$,

$$\mathcal{D} [\rho_1(t), \rho_2(t)] \equiv p_A(t).$$

It follows that the dynamics of the system is non-Markovian ($\mathcal{N} > 0$) if

$$\sigma(t) = \dot{p}_A(t) = \int dk \dot{\rho}_A(k, t) > 0$$

for some time $t$.

In Fig. 4, we plot the non-Markovianity witness $\sigma(t) = \dot{p}_A(t)$ found from numerical integration of Eq. (28) with the initial condition given in Eq. (15). A positive value of the witness $\sigma(t) = \dot{p}_A(t) > 0$ indicates non-Markovian dynamics (the walker returns to sublattice $A$ from the reservoir). The result in Fig. 4 is shown as a function of the reservoir bandwidth $\Delta$ and time $t$. Shaded regions clearly indicate non-Markovian evolution even in the topologically protected part of the phase diagram in Fig. 3(a) ($\alpha \leq 1$). This demonstrates that Markovianity is not essential for the topological transition. Furthermore, as one would intuitively expect, the evolution becomes more Markovian for larger bandwidth $\Delta$. In particular, for any fixed time $t$, Fig. 4 shows $\sigma \leq 0$ for sufficiently large bandwidth $\Delta$.

![FIG. 4. The non-Markovianity witness given in Eq. (45) $\sigma(t) = \dot{p}_A(t)$ as a function of the reservoir bandwidth $\Delta$ and time for $\alpha = 0.5$. In the blank region, $\sigma < 0$, whereas in the shaded regions $\sigma > 0$ and the evolution is non-Markovian. Here, $v > 0$, $J_0 v^{\alpha+1} = 0.01$, and $\alpha = 2$.](012215-7)

**VII. CONCLUSIONS AND OUTLOOK**

We have extended the analysis presented in Ref. [12] for Markovian non-Hermitian quantum walks by introducing an additional set of levels in each unit cell describing a reservoir that the walker may coherently enter and leave. The robust topological transition in the average walker displacement $\langle m \rangle$, previously found for the Markovian model, persists in the non-Markovian regime under appropriate conditions on the reservoir spectral density. The result is summarized in the phase diagram presented in Fig. 3. In particular, this phase diagram shows that for a sub-Ohmic or an Ohmic spectral density $[J(\epsilon) \sim \epsilon^\alpha$ with spectral exponent $\alpha \leq 1$], the walker decays into the reservoir in the long-time limit, and there is a robust topological transition; for a super-Ohmic spectral density ($\alpha > 1$), there is no transition. This difference in walker dynamics is directly related to the well-known localization transition in the spin-boson model [24].

To confirm that the walker dynamics is non-Markovian, we have numerically evaluated a non-Markovianity witness based on the Breuer measure [25] of non-Markovianity. In this problem, the non-Markovianity witness is positive whenever the walker reenters the lattice from the continuum. The result is shown in Fig. 4 where the dynamics is clearly non-Markovian even in a parameter regime with a robust topological transition.

In addition to a direct simulation of the quantum walk [Fig. 1(a)] through an array of, e.g., quantum dots, it may also be possible to experimentally realize the equivalent level structure shown in Fig. 1(b) with an alternative system that may be easier to engineer and control. For example, the starting Hamiltonian presented in Eqs. (4)–(6) is analogous to that used routinely in a STIRAP setup [27]. Alternatively, we have shown that the problem of the walker can be mapped to the Weisskopf-Wigner problem of atomic decay with a structured...
environment. In a recent work (Ref. [28]), Kriener et al. have simulated Weiskopf-Wigner dynamics with an engineered spectral density. Their implementation used ultracold atoms in an optical lattice, and they have observed non-Markovian dynamics in the system. Executing such an experiment with a range of parameters \( v(k) \) for \( k \in (0, \pi) \) would allow one to reconstruct the functional form of \( \rho_A(k) \) throughout the Brillouin zone. This would allow for an evaluation of the average walker displacement \( \langle m \rangle \) [see Eq. (13)]. If the experiment were reproduced for a range of spectral exponents \( \alpha \) and ratios \( u = v'/v \), the phase diagram shown in Fig. 3 could potentially be confirmed experimentally.

More broadly, this paper extends the notion of nonequilibrium topological phenomena to non-Markovian systems and stimulates the question: What new robust nonequilibrium phenomena may be found in non-Markovian open quantum systems?

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### APPENDIX A: AVERAGE DISPLACEMENT

We start from the definition of the average displacement given in Eq. (10). We apply the Fourier transform defined above Eq. (4), and we find

\[
\langle m(t) \rangle = \int \frac{dk}{\sqrt{2\pi}} \int \frac{dk'}{\sqrt{2\pi}} \left( \sum_{l \in \Lambda} \psi_l^{*}(k', t) \psi_l(k, t) \right)
\]

\[
\times \sum_m \left[ -i \partial_k e^{im(k-k')} \right]
\]

\[
= \int \frac{dk}{\sqrt{2\pi}} \int \frac{dk'}{\sqrt{2\pi}} \left( \sum_{l \in \Lambda} \psi_l^{*}(k', t) \left[ i \partial_k \psi_l(k, t) \right] \right)
\]

\[
\times \sum_m e^{im(k-k')} \]

\[
= i \int dk \sum_{l \in \Lambda} \psi_l^{*}(k, t) \partial_k \psi_l(k, t),
\]

where we integrated by parts. We now rotate away the phase \( \phi(k) \) associated with the Fourier transform of the coupling, \( v(k) = |v(k)| e^{i\phi(k)} \),

\[
H(k) \rightarrow \tilde{H}(k) = e^{i\Pi_A \phi(k)} H(k) e^{-i\Pi_A \phi(k)},
\]

where \( \Pi_A \) is the projector onto the \( \Lambda \) subspace,

\[
\Pi_A = \mathbf{1} - |A\rangle \langle A|.
\]

The states transform as

\[
|\psi(t)\rangle \rightarrow |\tilde{\psi}(t)\rangle = e^{i\Pi_A \phi(k)} |\psi(t)\rangle.
\]

Then, in this rotated frame, we find

\[
\langle m(t) \rangle = i \int dk \sum_{l \in \Lambda} e^{i\phi(l)} \tilde{\psi}_l^{*}(k, t) \partial_k [e^{-i\phi(k)} \tilde{\psi}_l(k, t)]
\]

\[
= i \int dk \sum_{l \in \Lambda} \tilde{\psi}_l^{*}(k, t) \partial_k \tilde{\psi}_l(k, t)
\]

\[
+ \int dk \sum_{l \in \Lambda} |\tilde{\psi}_l(k, t)|^2 \partial_k \phi(k).
\]

### APPENDIX B: SCHRIEFFER-WOLFF APPROXIMATION

We split the Hamiltonian \( H(k) \) into a diagonal term \( H_0(k) \), a term coupling \( B \) to \( A \) sites \( V(k, \text{Eq. (6)}) \), and a term coupling \( B \) and \( \{j\} \) sites \( V_g(k, \text{Eq. (6)}) \),

\[
H(k) = H_0(k) + V(k) + V_g(k),
\]

\[
H_0(k) = \epsilon_A |A, k\rangle \langle A, k| + (\epsilon_A + \omega)|B, k\rangle \langle B, k|
\]

\[
+ \sum_{j \in C} \epsilon_j |j, k\rangle \langle j, k|.
\]

\[
V_g(k) = \sum_{j \in C} g_j |j, k\rangle \langle B, k| + \text{H.c.}
\]

We rotate the Hamiltonian by means of an anti-Hermitian generator \( S \),

\[
H(k) \rightarrow e^S H(k) e^{-S}
\]

\[
= H(k) + [S, H(k)] + \frac{1}{2}[S, [S, H(k)]] + \cdots.
\]

We eliminate the coupling to \( B \) sites at first order by requiring \([S, H_0(k)] = -[V(k) + V_g(k)]\). Explicitly, \( S \) is given by

\[
S = \frac{\omega}{\omega} |A, k\rangle \langle B, k| - \text{H.c.}
\]

\[
- \sum_j g_j \langle j, k | B, k | - \text{H.c.}
\]

We keep only terms up to second order in \( V(k) \) and \( V_g(k) \) and project out site \( B \). The resulting Hamiltonian \( H_{SW}(k) \) has renormalized energies on sites \( A \) and \( \{j\} \) as well as a direct coupling between site \( A \) and levels \( \{j\} \).
We find

\[ H_{SW}(k) = H_0(k) + \frac{1}{2} [S, V(k)] + \frac{1}{2} [S, V_g(k)], \]  

(B6)

\[ = \tilde{\epsilon}_A(k)|A, k\rangle\langle A, k| + \sum_j \tilde{\epsilon}_j |j, k\rangle\langle j, k| \]

\[ + \sum_j \tilde{\eta}_j(k)|A, j, k\rangle\langle j, k| + \text{H.c.} \]

\[ + \sum_{j \neq j'} t_{j,j'}(k)|j, k\rangle\langle j', k| + \text{H.c.,} \]

(B7)

\[ \tilde{\epsilon}_A(k) = \epsilon_A - \frac{\langle v(k) \rangle^2}{\omega}, \]  

(B8)

\[ \tilde{\epsilon}_j = \epsilon_j - \frac{1}{2} \frac{|g_j|^2}{\epsilon_A + \omega - \epsilon_j}, \]  

(B9)

\[ \tilde{\eta}_j(k) = -\frac{\langle v(k) g_j^* \rangle}{2} \left( \frac{1}{\omega} + \frac{1}{\epsilon_A + \omega - \epsilon_j} \right), \]  

(B10)

\[ t_{j,j'} = -\frac{1}{2} \frac{g_j^* g_{j'}^*}{\epsilon_A + \omega - \epsilon_j}. \]  

(B11)

The coupling \( t_{j,j'} \) between levels in the reservoir will lead to a modification of the spectral density, in general. When a particular spectral density can be designed for the bare levels \( \{ j \} \), it may be advantageous to work in the limit of weak-coupling \( g_j \) and large \( \omega \) so that these corrections can be neglected. Alternatively, the reservoir could be re-diagonalized accounting for these corrections, and it may be possible to account for the associated change to the spectral density.

**APPENDIX C: GENERALIZED MASTER EQUATION**

We want to write a master equation for the probability density \( \rho_A(k, t) \) for finding the walker in sublattice \( A \) (having the atom in the excited-state \( A \) in the Weisskopf-Wigner model),

\[ \rho_A(k, t) = \text{Tr}[|A, k\rangle\langle A, k|\rho(t)], \]  

(C1)

where, here, we take \( \rho(t) \) to be the full density matrix in the enlarged (tensor product) Hilbert space of the Weisskopf-Wigner model. In this description, the Hilbert space of the walker (atom) is spanned by the states \( |A, k\rangle \) and \( |C, k\rangle \). The Hilbert space of the reservoir is spanned by states \( |0\rangle \) and \( |\{ j \}\rangle \) [Eqs. (21) and (22)].

We assume an initial tensor product state,

\[ \rho(0) = \rho_S(0) \otimes \rho_E(0), \]  

(C2)

where \( \rho_S(0) \) denotes the initial density matrix of the system (walker or atom) and \( \rho_E(0) \) is the initial density matrix of the environment, which we take to be

\[ \rho_E(0) = |0\rangle\langle 0|, \]  

(C3)

where state \( |0\rangle \) indicates the vacuum state of the environment with no photons.

We project out the degrees of freedom of the environment to obtain a master equation for the density matrix \( \rho_S(t) \) of the system. To accomplish this, we use the projection superoperator \( \mathcal{P} \), defined by its action on an operator \( \mathcal{O} \)

\[ \mathcal{P} \mathcal{O} = \rho_S(t) \otimes \text{Tr}_E \mathcal{O}, \]  

(C4)

where \( \text{Tr}_E \) is the partial trace over the environment: \( \text{Tr}_E[\mathcal{O}] \equiv \langle 0|\mathcal{O}|0\rangle + \sum_j \langle j|\mathcal{O}|j\rangle \). We also define the Liouvillian super-operators \( \mathcal{L}_S \) and \( \mathcal{L}_V \),

\[ \mathcal{L}_S \mathcal{O} = [H_S, \mathcal{O}], \]  

(C5)

\[ \mathcal{L}_V(t) \mathcal{O} = [V(t), \mathcal{O}], \]  

(C6)

where the system and coupling Hamiltonians in the Weisskopf-Wigner Hilbert space are defined by

\[ H_S = \int dk \langle C, k|\langle C, k| \otimes \sum_j \tilde{\epsilon}_j |j\rangle\langle j|, \]  

(C7)

\[ V(t) = \sum_j \int dk \tilde{\eta}_j(k)e^{-i\tilde{\epsilon}_j t}|A, k\rangle\langle C, k| \otimes |0\rangle\langle j| + \text{H.c..} \]  

(C8)

For the initial condition given in Eq. (C2), \( \mathcal{P} \) has the following properties:

\[ \mathcal{P}\rho(t) = \text{Tr}_E[\rho(t)] \otimes \rho_E(0), \]  

(C9)

\[ \mathcal{P}\rho(0) = \rho(0), \]  

(C10)

\[ \text{Tr}[|l, k\rangle\langle l, k|\mathcal{P}\rho(t)] = \text{Tr}[|l, k\rangle\langle l, k|\rho(t)] = \rho_S(k, t), \]  

(C11)

where \( l \in \{ A, C \} \).

Using these properties, and noting that \( \mathcal{P} \mathcal{L}_V \mathcal{P} = 0 \), the generalized master equation for \( \mathcal{P}\rho(t) \) in the interaction picture is given by [31]

\[ \frac{d}{dt} \tilde{\rho}(t) = -i \int_0^t dt' \Sigma(t, t') \mathcal{P}\tilde{\rho}(t'). \]  

(C12)

Here, \( \tilde{\rho}(t) \) is the density matrix in the interaction picture with respect to the system Hamiltonian,

\[ \tilde{\rho}(t) = e^{i\mathcal{E}t} \rho(t). \]  

(C13)

In the Born approximation, the self-energy \( \Sigma(t, t') \) is given by

\[ \Sigma(t, t') = -i \mathcal{P} \mathcal{L}_V(t) \mathcal{L}_V(t') \mathcal{P}. \]  

(C14)

Expanding Eq. (C14) in terms of commutators, we find

\[ \dot{\rho}_S(t) = -\int_0^t dt' \text{Tr}_E[[V(t'), [V(t'), \rho_S(t') \otimes \rho_E(0)]]]. \]  

(C15)

Evaluating the commutators and using

\[ \rho_A(k, t) = \langle A, k|\rho_S(t)|A, k\rangle, \]  

(C16)

we find Eqs. (23) and (24) in the main text.


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