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Optimal Dephasing for Ballistic Energy Transfer in Disordered Linear Chains

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We study the interplay between dephasing, disorder, and coupling to a sink on transport efficiency in a one-dimensional chain of finite length N, and in particular the beneficial or detrimental effect of dephasing on transport. The excitation moves along the chain by coherent nearest-neighbor hopping Ω, under the action of static disorder W and dephasing γ. The last site is coupled to an external acceptor system (sink), where the excitation can be trapped with a rate Γ_{trap}. While it is known that dephasing can help transport in the localized regime, here we show that dephasing can enhance energy transfer even in the ballistic regime. Specifically, in the localized regime we recover previous results, where the optimal dephasing is independent of the chain length and proportional to W or W^2/Ω. In the ballistic regime, the optimal dephasing decreases as $1/N$ or $1/\sqrt{N}$ respectively for weak and moderate static disorder. When focusing on the excitation starting at the beginning of the chain, dephasing can help excitation transfer only above a critical value of disorder W^{cr}, which strongly depends on the sink coupling strength Γ_{trap}. Analytic solutions are obtained for short chains.

I. INTRODUCTION

The optimization of excitonic and charge transport is a central problem for building quantum devices with different functions, including sensing, computing, and light-harvesting. Theoretically, the problem is challenging due to the interplay of different environments. Under low light intensity, in many natural photosynthetic systems or in ultra-precise photon sensors, the single-excitation approximation is usually valid. In this case the system is equivalent to a quantum network where one excitation can hop from site to site [1–5]. For a realistic description of the quantum transport problem, however, one has to consider not only the quantum coherent evolution, but also the coupling to multiple environments. These include an external acceptor system (sink), where the excitation can be donated and trapped, and the coupling with a phonon bath, which can induce different types of disorder: Static disorder (position dependent but time independent) and noise (time-dependent disorder).

From the study of natural photosynthetic complexes [6–10] has emerged the idea that in the optimal transport regime the energy scale of the coherent internal coupling is the same as the scale of the coupling to the external environment. This leaves little room for perturbative simplifications, and the analysis of the interplay of internal and external coupling must be carried out with care. Another important issue is related to finite-size effects. Indeed, many relevant natural and artificial quantum networks are made of a few two-level systems. For instance, the FMO complex in green sulphur bacteria, which is thought to have the role of a quantum wire, is made of eight bacteriochlorophyll a molecules [6]. The LHI and LHII [11] complexes in purple bacteria are made of 32 and 16–18 molecules, respectively. So the infinite system size limit also cannot be used to simplify the problem of exciton transport.

In a recent paper by the same authors [12], exciton transport in different quantum networks was considered in the semiclassical limit, focusing on the role of the coupling to the external acceptor system, which can induce coherent effects such as supertransfer of the excitation even in the presence of large dephasing. Here we focus our attention on the case of a linear chain of sites with nearest-neighbor coherent hopping of the excitation. Without invoking the semiclassical limit (where dephasing is large with respect to the coherent nearest-neighbor coupling), we analyze here the problem of optimal transport in the presence of dephasing, static disorder, and a coherent coupling to an external acceptor system. We focus on the role of dephasing noise (time-dependent perturbations) in enhancing transport, defined by the average transfer time. The interplay between dephasing and disorder was already studied in [13]. It is well known that noise is not always detrimental to transport and in some situations may enhance efficiency [13–15]. Specifically, noise-enhanced transport can occur whenever coherent effects, such as localization, subradiance, or another kind of destructive interference, are acting to suppress transport.

Several works in the literature aim to understand the parameter regime in which transport efficiency is maximized. Some general principles that might be used as a guide to understand how optimal transport can be achieved have been proposed: Enhanced noise assisted transport [14, 15], the Goldilocks principle [16], and superradiance in transport [17, 18].

Specifically, transport in one-dimensional chains has been studied in depth recently in the absence of coupling to a sink [1, 16, 19]. The results obtained for a one-dimensional chain of length N can be summarized as follows: In the presence of static disorder there may be a nonzero optimal dephasing γ^{opt} for transport. If we call W the strength of static disorder and Ω the coherent nearest-neighbor hopping, two main regimes have been identified previously. $i)$ For $W \gg \Omega$, where the localization length $\xi \leq 1$, we have $\gamma^{\mathrm{opt}} \propto W$, independent of Ω. $ii)$ For $\Omega/\sqrt{N} \ll W \ll \Omega$, where $1 \ll \xi \ll N$, we have nonlinear dependence on the disorder strength, $\gamma^{\mathrm{opt}} \propto W^2/\Omega$. Note that in both regimes the optimal dephasing is independent of N. On the other hand, the role of the coupling to the acceptor systems and the value of the critical disorder needed for dephasing to help transport have not been investigated fully.

In this paper and in the recent work [12] we consider simple paradigmatic models where exact analytical results can be obtained and general guiding principles can be extracted. Despite the simplicity of our model, we explicitly take into account the simultaneous action of two different types of noise (static and dynamical) and the coupling to the sink. This makes the model highly non-trivial and complex enough to extract general features that can apply also to more realistic systems.

Contrary to what one might expect, dephasing helps transport not only in the localized regime, when $\xi < N$, but also in the deep ballistic regime, when $\xi \gg N$, due to a competition between the effects of static and dynamic disorder on transport. This counterintuitive result can be explained considering that the average transfer time of the excitation to the external sink does not depend only on how quickly the excitation spreads along the chain, but also on how much time it spends on the last chain site. In the ballistic regime, the probability to be on the last site undergoes large fluctuations in time, which can be smoothed by dephasing, leading to an enhanced transfer efficiency. Indeed, for generic initial conditions, the excitation can be partially trapped even in the clean system, due to the structure of the closed-system eigenstates, as discussed for example in Ref. [19]. In such situations, dephasing will aid transport even in the absence of disorder.

Throughout, we consider the scenario where the excitation traverses the entire length of the chain, with the initial excitation placed at one end, and the coupling to the absorber at the other. In this case, dephasing can help transport

only above a critical minimal disorder W^{cr} which depends on the coupling to the acceptor system. We also find that in the deep ballistic regime the optimal dephasing γ^{opt} is not size-independent but decreases with the chain length N, up to a length determined by $N \approx \xi$, where the optimal dephasing becomes independent of N.

The paper is organized as follows: In Sec. II we define the transport model, including the effects of dephasing, disorder, and coupling to the acceptor system. In Sec. III we obtain analytic and numerical results for the simplest finite-length chains: $N = 2$ and $N = 3$. Then in Sec. IV we examine the behavior for general N and obtain two separate delocalized regimes where the optimal dephasing displays N-dependent behavior. We summarize our results in Sec. VI.

II. MODEL DESCRIPTION

We study the optimal dephasing for exciton energy transfer (EET) in linear chains in the presence of disorder. The time evolution of the closed system can be expressed as

$$i\hbar\dot{\rho}(t) = [H_{\mathrm{sys}}, \rho(t)] \,. \tag{1}$$

The system Hamiltonian is usually expressed in the site basis as

$$H_{\mathrm{sys}} = \sum_{i=1}^{N} \hbar\omega_i \, |i\rangle \langle i| + \sum_{l,m}^{N} J_{lm} \, |l\rangle \langle m| \,, \tag{2}$$

where we work in the single-exciton regime, with state $|i\rangle$ representing an excitation on site i only, $\hbar\omega_i$ are the site energies, and J_{lm} are the inter-site couplings. EET systems are open and connect to acceptor systems, which serve as sinks. In this paper, we take site N to be connected to the sink. The effects of the coupling to a sink are conventionally addressed by augmenting the system Hamiltonian with a non-Hermitian term:

$$-i\mathcal{W} = -i\frac{\Gamma_{\mathrm{trap}}}{2} \, |N\rangle \langle N| \,. \tag{3}$$

This treatment of the sink and the limits of its validity have been analyzed in Ref. [20]; the non-Hermitian term can be thought of as due to a coherent coupling of site N to a continuum of states (for instance to an infinite lead), where the continuum has a large energy band width with respect to the energy band width of the system.

Consequently the time evolution of the reduced density matrix ρ of the system will be described as

$$i\hbar\dot{\rho} = [H_{\mathrm{sys}}, \rho] - i\{\mathcal{W}, \rho\} \,. \tag{4}$$

EET systems are subject to background noise, which results in dephasing. We use the Haken-Strobl-Reineker (HSR) model [21] to describe the dephasing behavior of the system as

$$\dot{\rho}_{ij} = -\gamma(1 - \delta_{ij})\rho_{ij}. \tag{5}$$

Finally, the full system dynamics can be expressed as

$$\dot{\rho}_{ij} = -\frac{i}{\hbar}(H_{\mathrm{eff}} \, \rho - \rho \, H_{\mathrm{eff}}^{\dagger})_{ij} - \gamma(1 - \delta_{ij})\rho_{ij}, \tag{6}$$

where $H_{\mathrm{eff}} = H_{\mathrm{sys}} - i\mathcal{W}$ is the effective non-Hermitian Hamiltonian of the system.

The efficiency of EET can be measured by the total population trapped by the sink [15, 22]

$$\eta = \Gamma_{\mathrm{trap}} \int_0^\infty \rho_{NN}(t) \, dt \,, \tag{7}$$

and the average transfer time to the sink [14]

$$\tau = \Gamma_{\mathrm{trap}} \int_0^\infty t \, \rho_{NN}(t) \, dt / \eta \,. \tag{8}$$

In this paper, we neglect the fluorescence effect of excitons so that $\eta = 1$, and the average transfer time τ reduces to

$$\tau = \Gamma_{\mathrm{trap}} \int_0^\infty t\rho_{NN}(t) \, dt \,. \tag{9}$$
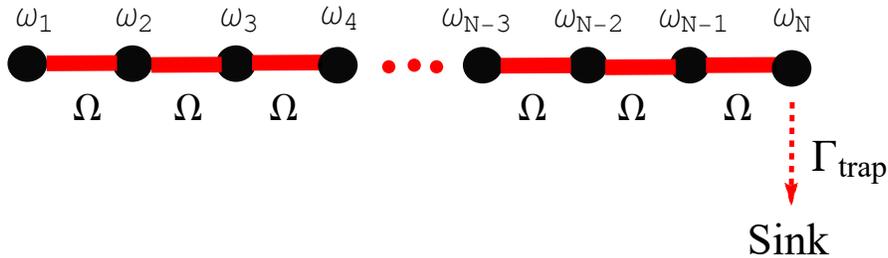
FIG. 1. (Color online) A schematic of a disordered linear chain that is attached to a sink.

We note that if decay via fluorescence is explicitly included, we have $\eta = 1/(1 + \Gamma_{\mathrm{fl}}\tau)$ for small fluorescence rate Γ_{fl} [23], and thus minimizing the transfer time τ is equivalent to maximizing the efficiency η.

Finally, if the master equation (6) is expressed in terms of the Liouville superoperator $\mathcal{L}$

$$\dot{\rho}(t) = -\mathcal{L}\rho(t), \tag{10}$$

we have

$$\tau = \frac{\Gamma_{\mathrm{trap}}}{\eta}(\mathcal{L}^{-2}\rho(0))_{\mathrm{NN}}. \tag{11}$$

In reality EET systems are often disordered. Here we consider Anderson-type disorder, with the site energies ω_i uniformly and independently distributed in the interval $[-W/2, W/2]$, where W denotes the disorder strength. The disorder-averaged transfer time is then calculated as

$$\langle\tau\rangle_W = \frac{1}{W^n}\int_{-W/2}^{W/2}\ldots\int_{-W/2}^{W/2}\tau(\omega_1, \omega_2, \ldots, \omega_n)\,d\omega_1\,d\omega_2\ldots d\omega_n. \tag{12}$$

For linear chains with uniform couplings, J_{lm} takes the form $J_{\mathrm{lm}} = \delta_{|l-m|,1}\Omega$, where Ω is the coupling constant. Furthermore, in the following we choose the initial state to be $\rho(0) = |1\rangle\langle 1|$ and set $\hbar = 1$ for simplicity.

III. OPTIMAL DEPHASING FOR TWO- AND THREE-SITE CHAINS

A. Explicit Solution and Optimal Dephasing for the 2-Site Model

For a two-site chain ($N = 2$), we have obtained in Ref. [12] a simple analytic form for τ by solving Eq. (11) exactly with $\rho(0) = |1\rangle\langle 1|$:

$$\tau_2 = \frac{1}{2\Omega^2}\left(\frac{4\Omega^2}{\Gamma_{\mathrm{trap}}} + \gamma + \frac{\Gamma_{\mathrm{trap}}}{2} + \frac{(\omega_1 - \omega_2)^2}{\gamma + \frac{\Gamma_{\mathrm{trap}}}{2}}\right), \tag{13}$$

where the subscript 2 here and in the following denotes the chain length. We now consider a disordered ensemble where the site energies ω_1 and ω_2 are uniformly and independently chosen from the interval $[-W/2, W/2]$. (Although the concept of disorder is normally applied to a large system, we will see that it is useful already in short chains, and allows for a straightofrward generalization to chains of arbitrary length.) After integration over disorder using Eq. (12), Eq. (13) becomes

$$\langle\tau_2\rangle_W = \frac{1}{2\Omega^2}\left(\frac{4\Omega^2}{\Gamma_{\mathrm{trap}}} + \gamma + \frac{\Gamma_{\mathrm{trap}}}{2} + \frac{W^2}{6(\gamma + \frac{\Gamma_{\mathrm{trap}}}{2})}\right). \tag{14}$$

We see from Eq. (14) that the average transfer time behaves monotonically with static disorder strength W, i.e., increasing disorder always slows down transport. On the other hand, there is a complex interplay between static
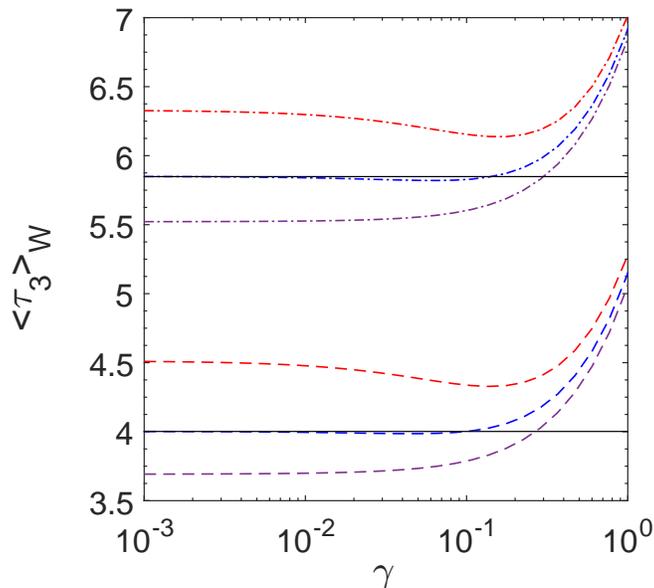
FIG. 2. (Color online) Plot of the average transfer time $\langle\tau_3\rangle_W$ as a function of dephasing rate γ for a 3-site chain. Here we fix the inter-site coupling $\Omega = 1$ while varying the coupling to the sink Γ_{trap} and disorder strength W. The three dashed curves are for $\Gamma_{\text{trap}} = 1$, and the three dot-dashed curves are for $\Gamma_{\text{trap}} = 10$; within each group from top to bottom we have $W = 1.5$, 1.1, and 0.7. Physically, the presence of a minimum for $W > 1$ indicates that appropriate dephasing can enhance the transport.

disorder W and dephasing γ, and this interplay depends in turn on the strength of the sink coupling Γ_{trap}. In particular, $\langle\tau_2\rangle_W$ has a minimum in γ when $W > W_2^{\text{cr}}$, where

$$W_2^{\text{cr}} = \sqrt{6}\Gamma_{\text{trap}}/2 \tag{15}$$

is the critical strength of disorder for a given coupling to the sink. Thus, dephasing can aid transport when disorder is sufficiently strong, $W > W_2^{\text{cr}}$, and dephasing will always retard transport when $W < W_2^{\text{cr}}$. In the regime $W > W_2^{\text{cr}}$, the optimal rate of dephasing is given exactly by

$$\gamma_2^{\text{opt}} = \frac{W}{\sqrt{6}} - \frac{\Gamma_{\text{trap}}}{2} = \frac{W - W_2^{\text{cr}}}{\sqrt{6}} \,. \tag{16}$$

B. The 3-site Chain – Symmetry between Large and Small Sink Coupling

For a chain of length $N = 3$, the exact transfer time τ_3 may be written down explicitly for a given realization of the disorder, for any dephasing rate and any coupling strength to the sink. The result, shown in Eq. (A1) in Appendix A, is unwieldy to work with analytically except in limiting cases; however it is easy to perform numerically the disorder integration given by Eq. (12). At first glance, the behavior is qualitatively similar to that of the $N = 2$ chain, as illustrated in Fig. 2. At fixed $\Omega = 1$ and weak disorder (small W), the transfer time τ_3 increases monotonically with dephasing rate γ, but as disorder increases, a minimum in γ appears and grows. The critical disorder in this case is seen numerically to be $W_3^{\text{cr}} \approx 1$ for both $\Gamma_{\text{trap}} = 1$ and $\Gamma_{\text{trap}} = 10$.

In Fig. 3, for each value of the sink coupling Γ_{trap} we calculate the ensemble-averaged transfer time $\langle\tau_3\rangle_W$ as a function of dephasing γ and disorder W, and obtain the disorder value W_3^{cr} at which τ_3 develops a minimum as a function of γ. Looking more closely at Fig. 3, we find an important qualitative difference in the system's behavior as compared with the 2-site case. For the 2-site chain, the critical disorder is always proportional to the sink coupling strength, $W_2^{\text{cr}} = \sqrt{6}\Gamma_{\text{trap}}/2$, regardless of the value of Ω. Now for the 3-site chain, the critical disorder is again proportional to the sink coupling Γ_{trap} for small coupling, but for large coupling the critical disorder *decreases* with the coupling strength. (More precisely, we have $W_3^{\text{cr}} = \Gamma_{\text{trap}}$ for $\Gamma_{\text{trap}} \ll \Omega$ and $W_3^{\text{cr}} = 6\sqrt{2}\Omega^2/\Gamma_{\text{trap}}$ for $\Gamma_{\text{trap}} \gg \Omega$, as will be obtained analytically below.)

The symmetry between large and small coupling to the sink is related to the superradiance transition in quantum systems coupled to a sink, where for sufficiently large coupling a segregation of resonances into superradiant states
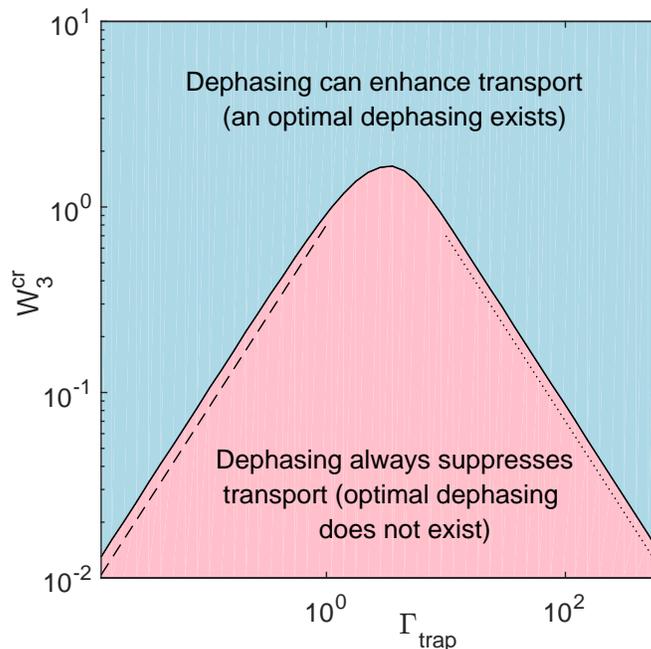
FIG. 3. (Color online) Plot of critical disorder strength W_3^{cr} as a function of sink coupling Γ_{trap} in a 3-site chain. The curve separates two transport regimes. In the upper region of the phase diagram (light blue), dephasing of the right strength will enhance transport while in the lower region (pink), dephasing always suppresses transport. The straight lines of slope $+1$ and -1 indicate the scaling for small and large Γ_{trap}, respectively. Here we fix units where $\Omega = 1$.

(strongly coupled to the sink) and subradiant states (trapped away from the sink) occurs, with the result that escape to the sink is suppressed [24, 25]. Transport to the sink in the clean quantum system is maximized at the superradiance transition. In the case of the clean $N-$site chain (with no disorder or dephasing), the transfer time is given by

$$\tau = \frac{N}{\Gamma_{\mathrm{trap}}} + \frac{(N-1)\Gamma_{\mathrm{trap}}}{4\Omega^2}\,, \tag{17}$$

see, e.g., Ref. [12], and thus transport to the sink is optimized at $\Gamma_{\mathrm{trap}} = 2\sqrt{N/(N-1)}\Omega$, or $\Gamma_{\mathrm{trap}} = \sqrt{6}\Omega$ for $N = 3$.

1. Analytics for Weakly Coupled Sink

We now obtain analytically the critical disorder for the 3-site chain. We break up the problem into two regimes, starting with the regime of weak coupling to the sink: $\Gamma_{\mathrm{trap}} \ll \Omega$. After expanding τ_3 from Appendix A in powers of Ω^{-1} assuming Ω is large compared to all other energy scales in the problem, and integrating the expanded expression over disorder using Eq. (12), we obtain

$$\langle \tau_3 \rangle_W = \frac{3}{\Gamma_{\mathrm{trap}}} + \Omega^{-2} \left(\frac{3\gamma}{2} + \frac{\Gamma_{\mathrm{trap}}}{2} - \frac{W^2}{12\left(2\gamma + \Gamma_{\mathrm{trap}}\right)} + \frac{5W^2}{12\left(4\gamma + \Gamma_{\mathrm{trap}}\right)} \right) + O\left(\Omega^{-4}\right). \tag{18}$$

Differentiating $\langle \tau_3 \rangle_W$ with respect to γ, and neglecting $O(\Omega^{-4})$ terms, we find

$$\frac{\partial \langle \tau_3 \rangle_W}{\partial \gamma} \approx \frac{1}{12\Omega^2} \left[18 + W^2 \left(\frac{2}{\left(2\gamma + \Gamma_{\mathrm{trap}}\right)^2} - \frac{20}{\left(4\gamma + \Gamma_{\mathrm{trap}}\right)^2} \right) \right]. \tag{19}$$

Now $\frac{2}{(2\gamma + \Gamma_{\mathrm{trap}})^2} - \frac{20}{(4\gamma + \Gamma_{\mathrm{trap}})^2}$ is always negative for non-negative γ and Γ_{trap}. Furthermore, the quantity in square brackets in Eq. (19) increases monotonically from $18(1 - W^2/\Gamma_{\mathrm{trap}}^2)$ to 18 as γ increases from 0 to ∞. Thus for $W < \Gamma_{\mathrm{trap}}$, Eq. (19) is always positive, and dephasing always retards transport. For $W > \Gamma_{\mathrm{trap}}$, on the other hand,

Eq. (19) increases monotonically in γ from below 0 to above 0, i.e., the mean transfer time $\langle\tau_3\rangle_W$ exhibits a minimum as a function of γ. Thus, the critical disorder strength for weak sink coupling is given by

$$W_3^{\mathrm{cr}} = \Gamma_{\mathrm{trap}} . \tag{20}$$

What about the optimal dephasing γ_3^{opt}? As a function of disorder strength W when $W > W_3^{\mathrm{cr}}$, this is given in general by the solution of a quartic equation. Nevertheless, three relatively simple regimes may be distinguished, the first two of which fall within the range of validity of the large-Ω approximation, Eq. (18).

(i) For weak disorder only slightly above the critical value, $0 < W - W^{\mathrm{cr}} \ll W^{\mathrm{cr}}$, we may expand Eq. (19) and obtain $\gamma_3^{\mathrm{opt}} \approx \frac{9}{38}(W - W_3^{\mathrm{cr}})$.

(ii) For moderate disorder, $W^{\mathrm{cr}} \ll W \ll \Omega$, γ^{opt} will be large compared to $W_3^{\mathrm{cr}} = \Gamma_{\mathrm{trap}}$, and thus we may take $\gamma \gg \Gamma_{\mathrm{trap}}$ in Eq. (19). We then have $\gamma_3^{\mathrm{opt}} \approx W/2\sqrt{6}$.

(iii) Finally, one may consider the behavior for strong disorder, $W_3^{\mathrm{cr}} \ll \Omega \ll W$. This is outside the range of validity of the above derivation, since Ω is no longer the largest energy scale. In this parameter regime, to be discussed further in Sec. IV B, the optimal dephasing rate converges to the N-independent form $\gamma^{\mathrm{opt}} \approx W/\sqrt{6}$.

Interestingly, in each of the three ranges of the disorder strength W, the optimal dephasing rate γ_3^{opt} grows linearly with W, but the coefficient is different in each case. In Sec. IV B, we will see that each of the three regimes identified here for $N = 3$ has a counterpart at large N, but each is associated with a different scaling with system size N.

2. Analytics for Strongly Coupled Sink

Now we consider the scenario of strong coupling to the sink, $\Gamma_{\mathrm{trap}} \gg \Omega$. As far as the scaling analysis is concerned, a strongly coupled sink can be thought as a weakly coupled sink with the effective coupling strength $\Gamma'_{\mathrm{trap}} = \Omega^2/\Gamma_{\mathrm{trap}}$. So starting from the exact expression for τ_3 in Appendix A, we may change variables from Γ_{trap} to Γ'_{trap}, and expand τ_3 assuming Ω is very large (compared to all ω_i, γ, and Γ'_{trap}). Integrating over disorder, we obtain

$$\langle\tau_3\rangle'_W = \frac{1}{2\Gamma'_{\mathrm{trap}}} + \frac{18\left(\gamma + 2\Gamma'_{\mathrm{trap}}\right) + \frac{W^2}{\gamma + 2\Gamma'_{\mathrm{trap}}}}{\Omega^2} + O\left(\frac{1}{\Omega^4}\right) . \tag{21}$$

Straightforward algebra now shows that for strong sink coupling the critical disorder is given by

$$W_3^{\mathrm{cr}} = 6\sqrt{2}\Gamma'_{\mathrm{trap}} = 6\sqrt{2}\Omega^2/\Gamma_{\mathrm{trap}} , \tag{22}$$

and the optimal dephasing rate above critical disorder is seen to be

$$\gamma_3^{\mathrm{opt}} = (W - W_3^{\mathrm{cr}})/3\sqrt{2} . \tag{23}$$

IV. OPTIMAL DEPHASING FOR LONG CHAINS

A. Critical Disorder Strength for Long Chains

We now consider how the results obtained above for 2- and 3-site chains may extend to chains of general length N. To begin with, we generalize the results of Fig. 3 to N sites. Once again, without loss of generality we choose units where hopping $\Omega = 1$ and evaluate numerically, as a function of sink coupling Γ_{trap}, the critical disorder W^{cr} at which the ensemble-averaged transfer time $\langle\tau(\gamma)\rangle_W$ develops a minimum as a function of dephasing rate γ. For general N, Monte Carlo integration is used to evaluate the disorder average. The results, for selected values of N, are shown in Fig. 4. We notice in Fig. 4 the same qualitative behavior observed earlier in Fig. 3 for the 3-site chain. Furthermore, we see empirically that the behavior becomes N-independent for large N when the rescaled disorder strength $N^2 W^{\mathrm{cr}}$ is plotted as a function of Γ_{trap}, indicating that the critical disorder scales as

$$W^{\mathrm{cr}} \sim \frac{1}{N^2} \tag{24}$$

for all values of Γ_{trap}. In particular, comparing with the results for $N = 3$, we have

$$W^{\mathrm{cr}} \sim \frac{\Gamma_{\mathrm{trap}}}{N^2} \tag{25}$$
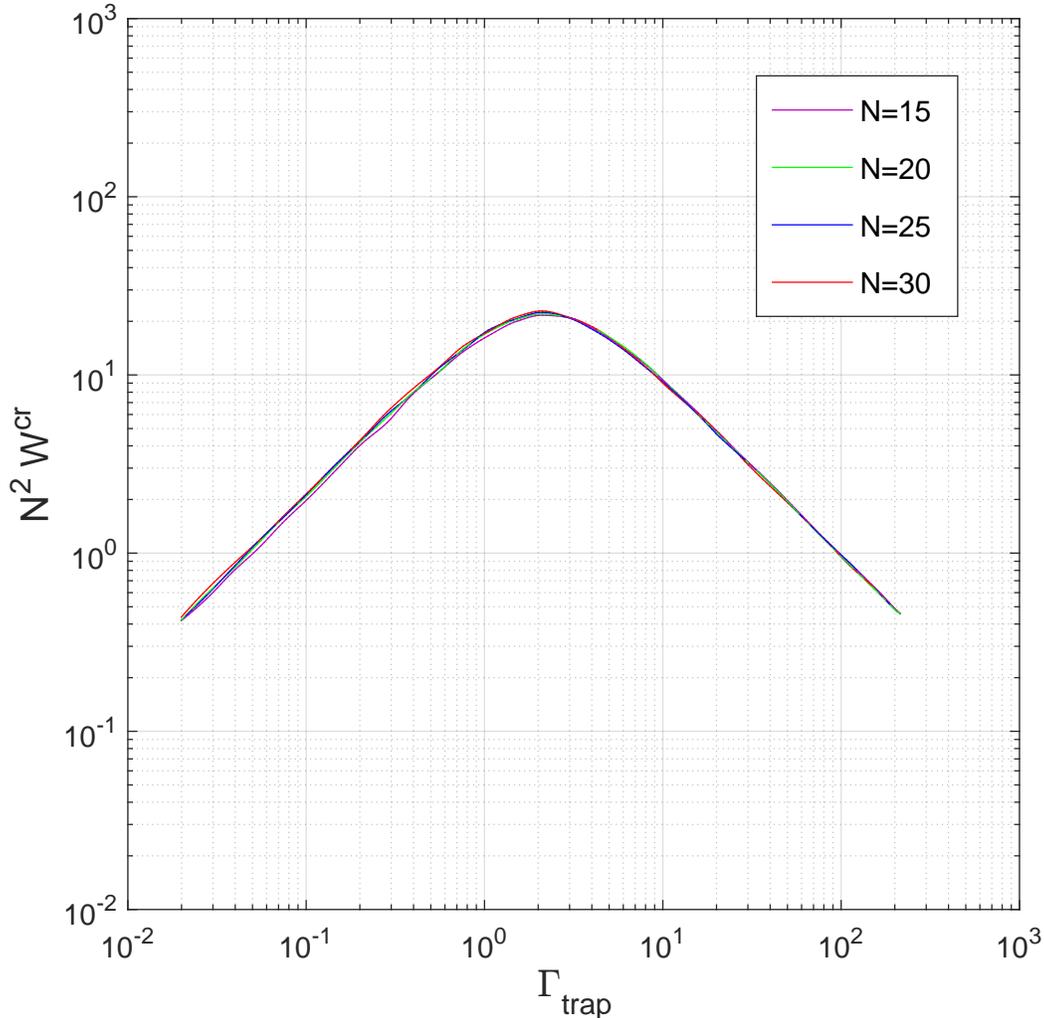
FIG. 4. (Color online) Plot of the rescaled critical disorder N^2W^{cr} as a function of sink coupling Γ_{trap} for various chain lengths N. Here we fix $\Omega = 1$.

for a weakly coupled sink, $\Gamma_{trap} \ll \Omega$, and

$$W^{cr} \sim \frac{\Omega^2}{N^2\Gamma_{trap}} \tag{26}$$

for a strongly coupled sink, $\Gamma_{trap} \gg \Omega$.

We notice that W^{cr} approaches zero as the chain length N goes to infinity. This is consistent with the fact that for an infinitely long chain, the system is localized at arbitrarily weak disorder, and any amount of dephasing can break the localization, thus aiding transport.

Unfortunately, an analytic understanding of the empirical scaling behavior (24) is not presently available; the analysis would require a non-perturbative treatment of the effect of the coupling Γ_{trap}, since near critical disorder Γ_{trap} will be comparable to both disorder W and dephasing strength γ.

B. Optimal dephasing as a function of disorder

We now consider the optimal dephasing for long chains when $W > W^{cr}$. Numerical results for three values of Γ_{trap} (one corresponding to weak coupling, another to strong coupling, and the third to a coupling right at the
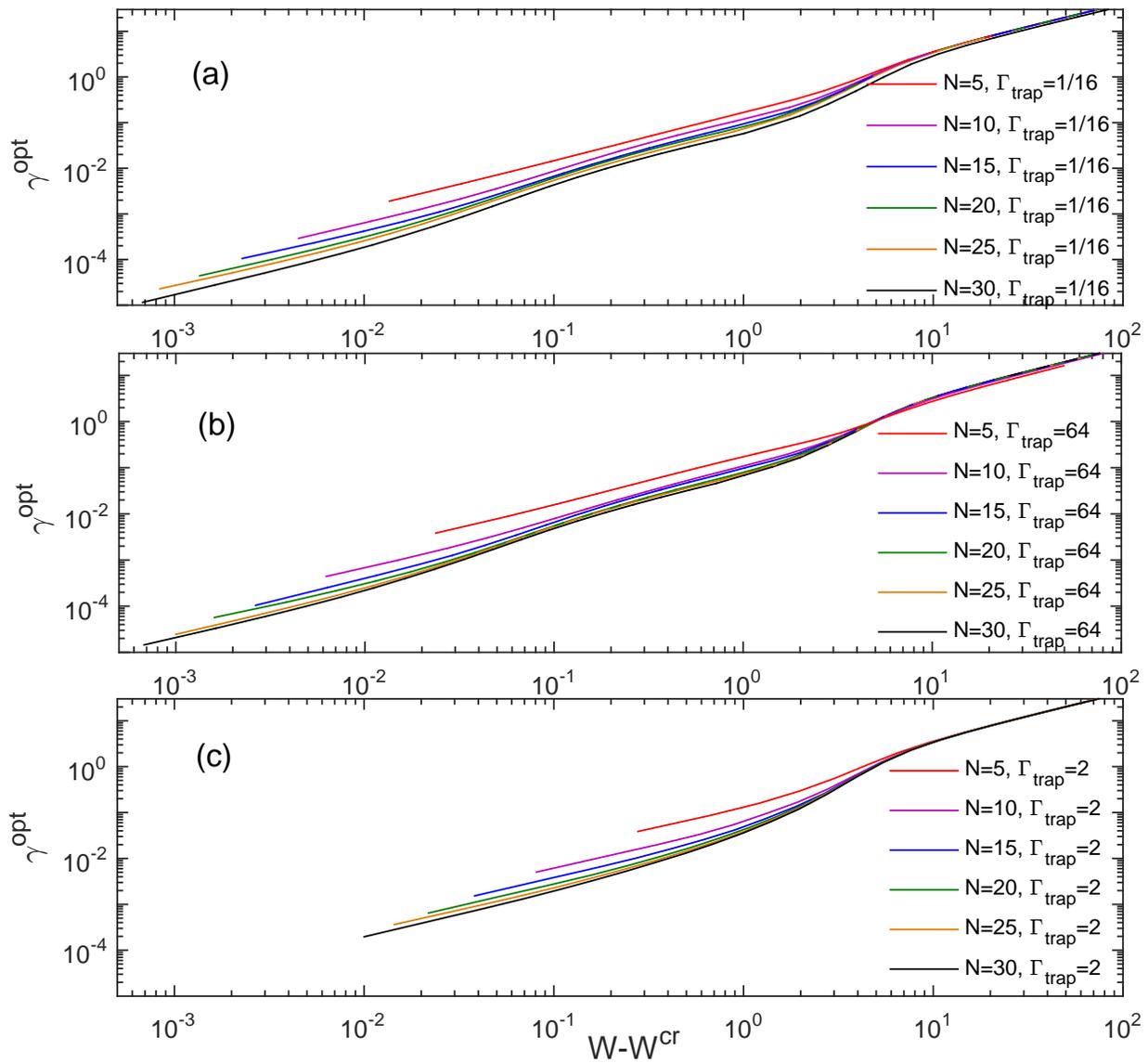
FIG. 5. (Color online) Optimal dephasing rate γ^{opt} is plotted as a function of $W - W^{\mathrm{cr}}$ for chains of different length N, where in each curve the minimum value of W is $1.4W^{\mathrm{cr}}$ and the critical disorder W^{cr} is itself a function of N. Here we again fix $\Omega = 1$. Panels (a) and (b) show results for $\Gamma_{\mathrm{trap}} = 1/16$ and 64, providing examples respectively of the weak-coupling and strong-coupling wings in Fig. 4. In each case, three distinct regimes may be observed for weak, moderate, and strong disorder, which display different scaling behavior with N and are analyzed in Secs. IV B 1, IV B 2, and IV B 3, respectively. Panel (c) shows results at the superradiance transition, $\Gamma_{\mathrm{trap}} = 2$; here the moderate disorder regime is absent.

superradiance transition), are shown in Fig. 5. We see that the optimal dephasing increases monotonically with the disorder strength. However, several distinct parameter regimes can be identified, which are in direct correspondence with the three regimes obtained for $N = 3$ in Sec. III B 1. Notably, each regime shows its own scaling behavior with the chain length N, even though this scaling is not clearly visible in Fig. 5. We now proceed with an analysis of the different regimes and their scaling behaviors.
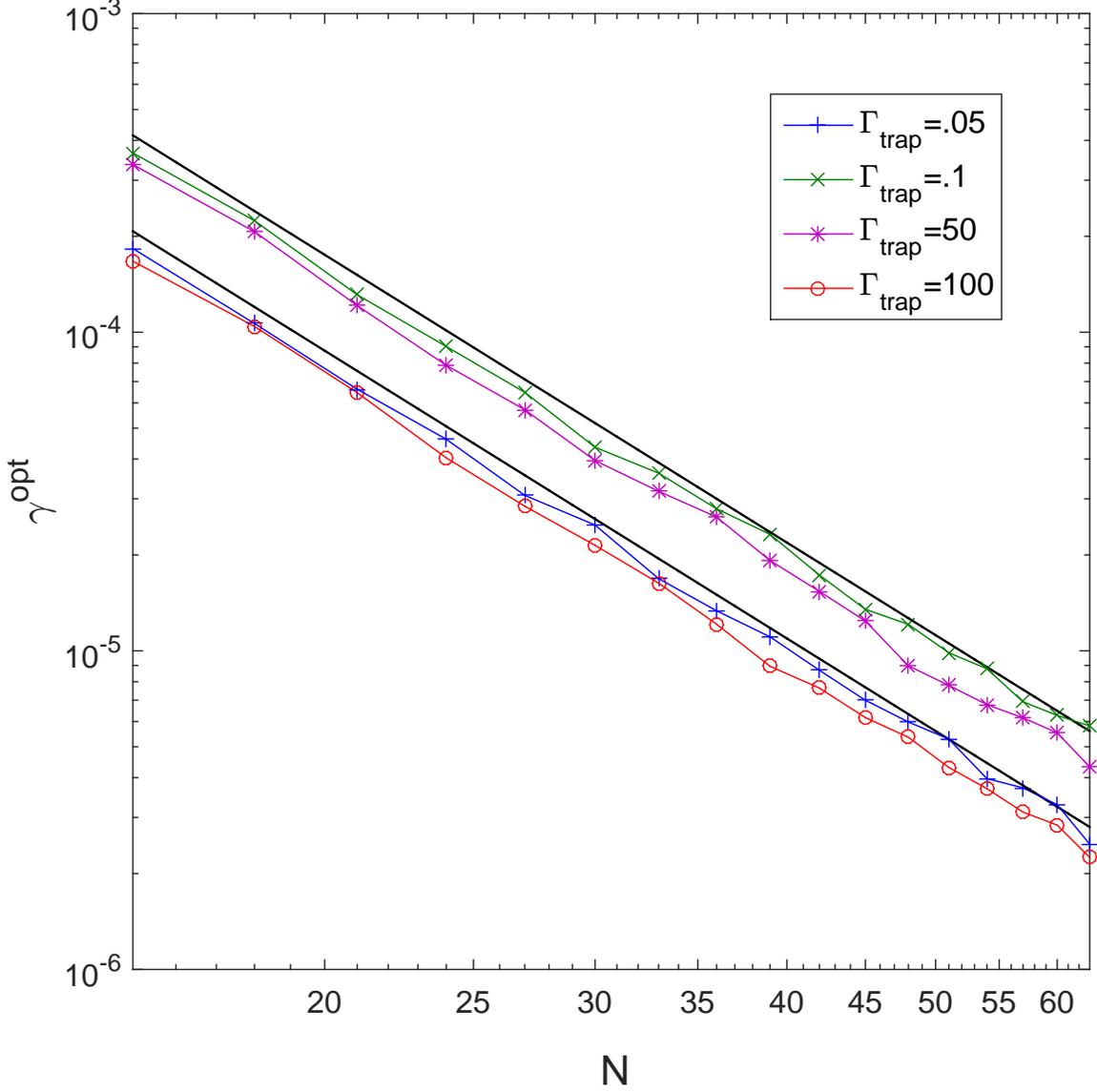
FIG. 6. (Color online) Optimal dephasing rate γ^{opt} is shown as a function of N with $W = 2W^{\mathrm{cr}}$ for several values of the sink coupling strength Γ_{trap}. Here $\Omega = 1$. The two black solid lines illustrate scaling proportional to $1/N^3$, implying $\gamma^{\mathrm{opt}} \sim (W - W^{\mathrm{cr}})/N$ for W close to W^{cr}.

1. Weak Disorder: $W - W^{\mathrm{cr}} \sim W^{\mathrm{cr}}$

We first consider W just slightly above the critical disorder, $0 < W - W^{\mathrm{cr}} \sim W^{\mathrm{cr}}$. As seen in Fig. 5, here the optimal disorder γ^{opt} grows linearly with $W - W^{\mathrm{cr}}$, just as it does for $N = 2$ and $N = 3$. To ascertain the N-dependence for long chains, in Fig. 6 we study γ^{opt} as a function of N for $W = 2W^{\mathrm{cr}}$ and several (large and small) values of the sink coupling strength Γ_{trap}. We observe the scaling $\gamma^{\mathrm{opt}} \sim 1/N^3$ when other parameters are held fixed, which combined with Eq. (24) implies

$$\gamma^{\mathrm{opt}} \sim \frac{W - W^{\mathrm{cr}}}{N} . \tag{27}$$
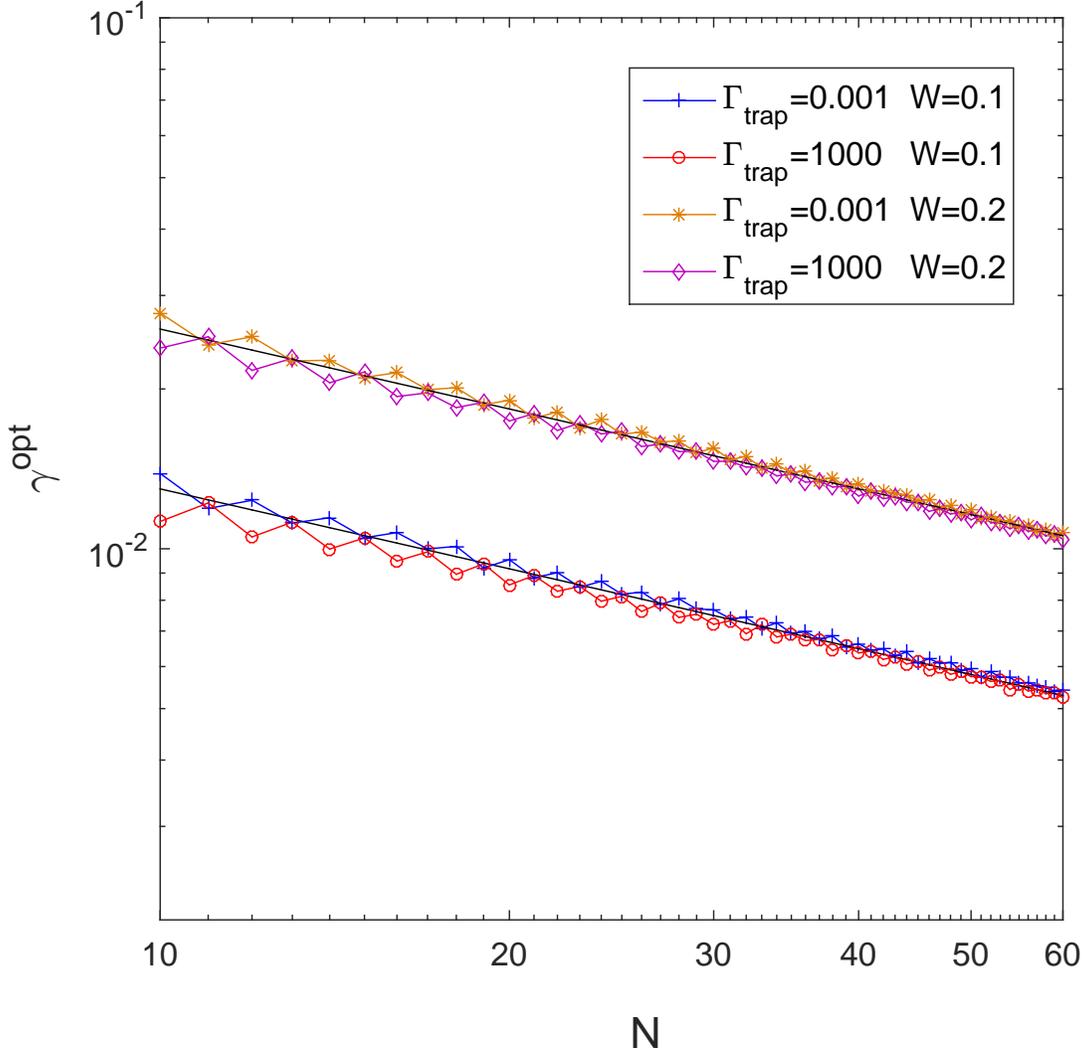
FIG. 7. (Color online) Optimal dephasing γ^{opt} is shown as a function of chain length N in the moderate-disorder regime, for several values of the sink coupling Γ_{trap} and disorder strength W. Here $\Omega = 1$. We observe good agreement with Eq. (30), as shown by the solid lines.

2. Moderate Disorder: $\Gamma_{\mathrm{trap}}/\sqrt{N} \ll W \ll \Omega/\sqrt{N}$

Here we consider the behavior where disorder (and dephasing) are strong compared to the sink coupling but still weak compared to the hopping amplitude. Thus, we are interested in the regime $\Gamma_{\mathrm{trap}} \ll W \sim \gamma \ll \Omega$ where any required N dependence is temporarily omitted from the inequalities.

It is convenient to begin with a clean chain coupled to a sink in the presence of dephasing. Here the transfer time may be obtained exactly as

$$\tau = \frac{N}{\Gamma_{\mathrm{trap}}} + \frac{N(N-1)\gamma + (N-1)\Gamma_{\mathrm{trap}}}{4\Omega^2}, \tag{28}$$

to be compared with Eq. (17) for the special case $\gamma = 0$. Now we consider expanding in both disorder strength W and sink coupling Γ_{trap} assuming that Γ_{trap} is small compared to Ω (i.e., we work in a regime analogous to that considered in Sec. III B 1 for $N = 3$; an analogous treatment for $\Gamma_{\mathrm{trap}} \gg \Omega$ may be considered as in Sec. III B 2). Beginning with Eq. (28) for $W = 0$ and comparing with the results (14) and (18) for $N = 2$ and 3 respectively, we conjecture that

for large N the expansion takes the form

$$\langle \tau \rangle_W = \frac{N}{\Gamma_{\text{trap}}} + \frac{1}{\Omega^2} \left[\left(\frac{N(N-1)}{4}\gamma + a(N)\frac{W^2}{\gamma} \right) + \Gamma_{\text{trap}} \left(\frac{N-1}{4} - b(N)\frac{W^2}{\gamma^2} \right) + O\left(\Gamma_{\text{trap}}^2\right) \right]$$
$$+ \frac{1}{\Omega^4} \left[c(N)W^2\gamma + d(N)\frac{W^4}{\gamma} + O(\Gamma_{\text{trap}}) \right] + O\left(\frac{1}{\Omega^6} \right) . \tag{29}$$

Numerically, we find $a(N) = a_0 N$, $b(N) = b_0$, $c(N) = c_0 N^3$, and $d(N) = d_0 N^2$ for large N. In particular, $a_0 \approx 0.042$.

For sufficiently large Ω and small Γ_{trap} we may restrict our attention to the term $\left(\frac{N(N-1)}{4}\gamma + a_0 N \frac{W^2}{\gamma} \right)/\Omega^2$ only, which implies that the optimal dephasing in this regime should behave as

$$\gamma^{\text{opt}} \approx \frac{2\sqrt{a_0}\,W}{\sqrt{N}} \approx 0.41 \frac{W}{\sqrt{N}} . \tag{30}$$

This predicted behavior with system size N for moderate disorder strength is confirmed in Fig. 7. We observe in Fig. 7 that while Eq. (30) was obtained in the context of $\Gamma_{\text{trap}} \ll \Omega$, the same scaling behavior, $\gamma^{\text{opt}} \sim 1/\sqrt{N}$, holds also for $\Gamma_{\text{trap}} \gg \Omega$ where the effective coupling to the sink $\Omega^2/\Gamma_{\text{trap}}$ is small.

Now to understand the range of validity of Eq. (30), we need to take a closer look at the two expansions in Eq. (29). On the one hand, our approximation breaks down for small disorder and dephasing when the terms proportional to Γ_{trap} become comparable to the Γ_{trap}-independent terms we have been considering. This occurs when $\gamma^{\text{opt}} \sim \Gamma_{\text{trap}}/N$, or equivalently $W \sim \Gamma_{\text{trap}}/\sqrt{N}$. On the other hand, the approximation also breaks down for larger disorder (and dephasing), when the $1/\Omega^4$ contribution becomes comparable to that of the $1/\Omega^2$ terms in the expansion. This occurs when $W \sim \Omega/\sqrt{N}$, which not coincidentally corresponds to the localization border where the localization length near the middle of the energy band, $\xi \approx 100\,\Omega^2/W^2$ [26], becomes comparable to the chain length N.

Thus the moderate-disorder regime in which the scaling of the optimal dephasing rate is given by Eq. (30) extends over the range $\Gamma_{\text{trap}}/\sqrt{N} \ll W \ll \Omega/\sqrt{N}$. We note that in the moderate-disorder regime as well as in the weak-disorder regime, the eigenstates are delocalized and wave packet motion is ballistic. Nevertheless, in both regimes we have shown that dephasing will aid transport.

3. Strong disorder: $W \gg \Omega/\sqrt{N}$

Finally, in the strong disorder regime, defined by $W \gg \Omega/\sqrt{N}$, the quantum eigenstates are localized, and the dynamics is diffusive. This regime has previously been studied in the absence of coupling to a sink in Refs. [1, 16, 19]. More precisely, this regime comprises two sub-regimes: For $\Omega/\sqrt{N} \ll W \ll \Omega$, one has $1 \ll \xi \ll N$, and the optimal dephasing rate is given by $\gamma^{\text{opt}} \sim \Omega/\xi \sim W^2/\Omega$. Upon further increase of the disorder, we reach $W \gg \Omega$, implying a localization length $\xi \sim 1$, and the optimal dephasing is then simply proportional to the disorder: $\gamma^{\text{opt}} \sim W$. Throughout the strong-disorder regime, the optimal dephasing is controlled by motion on the scale of a localization length, and as a consequence γ^{opt} is N-independent.

Specifically, for $W \gg \Omega$, the Leegwater classical-like approximation applies [27], and the transfer time is given by [12]

$$\langle \tau_{\text{L}} \rangle_W = \frac{N}{\Gamma_{\text{trap}}} + \frac{N(N-1)}{4\Omega^2} \left[\gamma + \frac{\Gamma_{\text{trap}}}{N} + \frac{W^2}{6\gamma} \left(1 - \frac{2\Gamma_{\text{trap}}}{N(2\gamma + \Gamma_{\text{trap}})} \right) \right] . \tag{31}$$

The optimal dephasing in this regime is

$$\gamma^{\text{opt}} \approx \frac{W}{\sqrt{6}} . \tag{32}$$

In Fig. 8 we examine explicitly the crossover between the moderate-disorder regime, where motion is ballistic and γ^{opt} scales with N in accordance with Eq. (30), and the strong-disorder regime where localization obtains and γ^{opt} becomes N-independent.

V. DISCUSSION

An interesting feature of our analysis is the fact that in a finite chain, dephasing can help transport even in the deep ballistic regime ($\xi \gg N$), where the spreading of the excitation is very fast and not only in the localized regime ($\xi \ll N$), as already discussed in many publications.
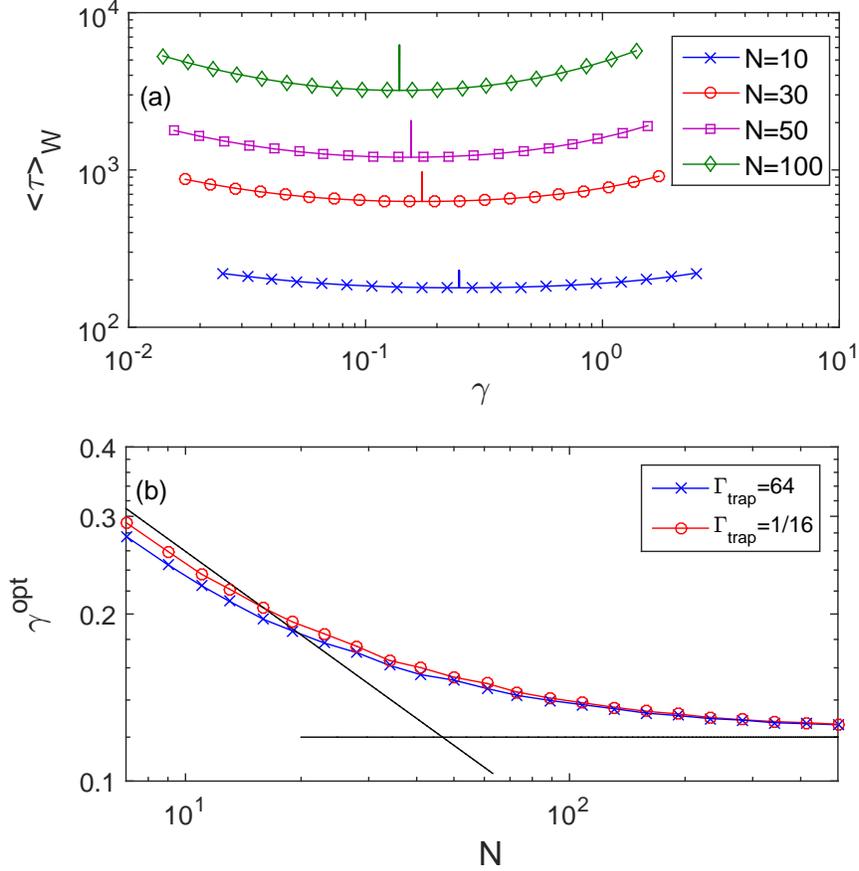
FIG. 8. (Color online) (a) The disorder-averaged transfer time $\langle\tau\rangle_W$ is shown as a function of dephasing rate γ for chains of several lengths N. Here $\Omega = 1$, $W = 2$, and $\Gamma_{\mathrm{trap}} = 1/16$. In each case, the vertical line indicates the optimal dephasing rate γ^{opt}. (b) The optimal dephasing γ^{opt} is shown as a function of chain length N in the crossover between the moderate-disorder and strong-disorder regimes. Here $\Omega = 1$, $W = 2$, and two values of the sink coupling Γ_{trap} are presented, corresponding to the weakly and strongly coupled sink scenarios. The solid lines represent Eq. (30) in the moderate-disorder regime (which displays $N^{-1/2}$ scaling) and the N-independent behavior expected for strong disorder.

Understanding how dephasing can help transport in the localized regime is not difficult. Here transport is suppressed in the absence of dephasing, and the excitation spreads only up to a length ξ, whereas nonzero dephasing frees the excitation leading to a diffusive spreading at large times. Thus, in this regime the spreading of the excitation is much faster in the presence of dephasing than without it.

In the ballistic regime, on the other hand, dephasing can even slow down the spreading of the excitation (indeed when dephasing is sufficiently large, it induces a diffusive spreading in a long chain which is much slower than the ballistic transport associated with zero dephasing). Nevertheless the efficiency of the energy transfer depends not only on the rate of excitation spreading, but also on the probability to be on the last site, which is coupled to the sink. In the clean case coherences induce large fluctuations in this probability as shown in Fig. 9(a), in contrast with the case of nonzero dephasing where the fluctuations are smoothed so that that on average the excitation spends more time on the last site, thus increasing the transfer efficiency. This enhancement due to dephasing can happen even if the rate of excitation spreading is the same without or with dephasing, as seen in the initial linear growth of the spreading $\sigma(t)$ in Fig. 9(b). Of course, too high a rate of dephasing for a given chain length and a given strength of static disorder will suppress transport, turning ballistic spreading into diffusive. Nevertheless for any finite size chain, there is always a finite optimal dephasing even in the ballistic regime.

Finally we would like to stress that in this paper we have focused on the case of the excitation starting from the first site. Here we found that dephasing can help only above a critical static disorder. On the other hand, starting from other initial conditions, dephasing can help energy transfer even in the absence of static disorder. For instance for a three-site chain with $W = 0$ (the clean case), when the excitation starts from the middle site, the transfer time
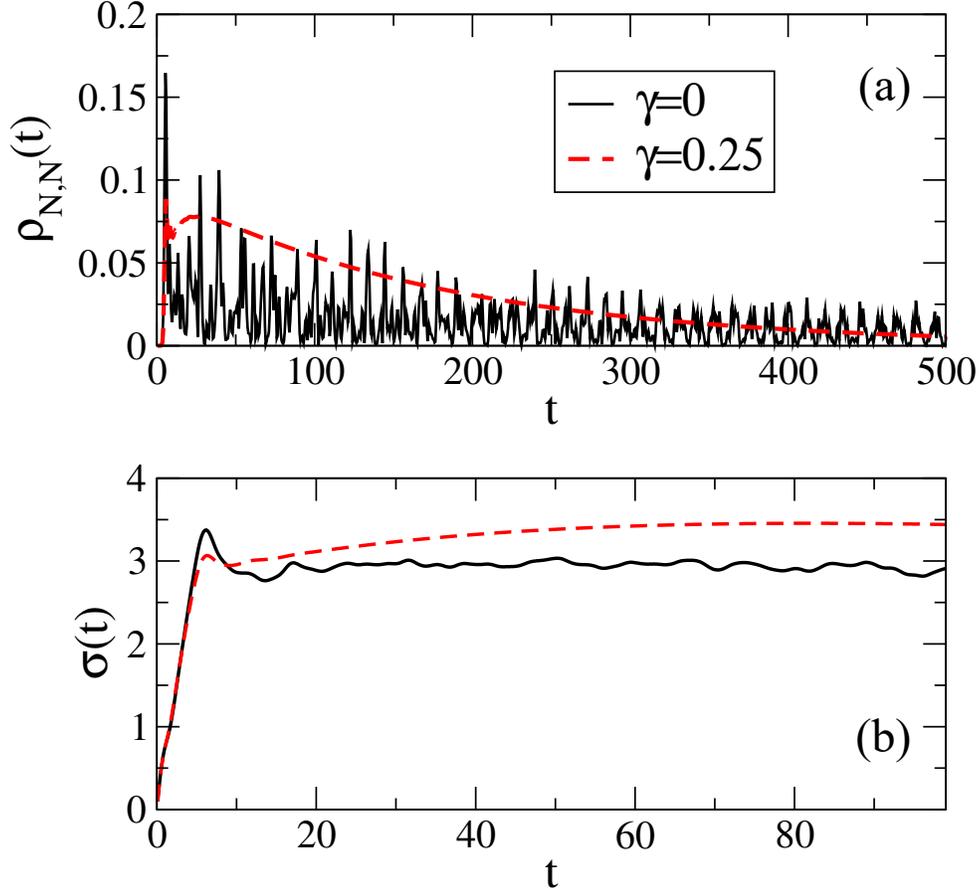
FIG. 9. (Color online) (a) Probability to be at site N as a function of time, for an excitation initially at site 1. Here $\Omega = 1$, $W = 2$, $N = 10$, and $\Gamma_{\text{trap}} = 1/16$ as in Fig. 8. The data refer to a single disorder realization without dephasing (solid black curve) and at the optimal dephasing, $\gamma \approx 0.25$ (red dashed curve). (b) Excitation spreading $\sigma(t)$ for the same parameters as in panel (a). Here an average is performed over 100 disorder realizations. Note that the spreading is defined as: $\sigma^2(t) = \sum_n \rho_{n,n}(t)n^2 - (\sum_n \rho_{n,n}n)^2$.

is analytically given by

$$\tau = \frac{3}{\Gamma_{\text{trap}}} + \frac{1}{2\gamma + \Gamma_{\text{trap}}} + \frac{2\gamma + \Gamma_{\text{trap}}}{2\Omega^2}, \tag{33}$$

which gives an optimal dephasing $\gamma^{\text{opt}} = (\sqrt{2}\Omega - \Gamma_{\text{trap}})/2$ even in the absence of any static disorder. More generally, when the excitation starts in the middle of a clean chain of length N, for N odd, in the limit of weak coupling Γ_{trap} ($\Gamma_{\text{trap}} \ll \Omega, \gamma$) we observe that

$$\tau = \frac{N}{\Gamma_{\text{trap}}} + \frac{1}{2\gamma} + \frac{(3N^2 - 4N + 1)\gamma}{16\Omega^2}, \tag{34}$$

and the optimal dephasing is therefore given by

$$\gamma^{\text{opt}} = \frac{\sqrt{8}\Omega}{\sqrt{3N^2 - 4N + 1}} + O(\Gamma_{\text{trap}}), \tag{35}$$

which falls off as Ω/N for long chains. A more detailed investigation of the role of noise in the absence of static disorder and the dependence on initial conditions will be done elsewhere. For the moment we only comment that Eqs. (33) and (34) confirm the key result, which is that even in the ballistic regime dephasing can help energy transfer, in a finite-size system.

VI. CONCLUSIONS

We have systematically studied the effect of dephasing on transport in disordered chains of arbitrary length coupled to a sink. Specifically, we have considered a linear chain of N sites with nearest-neighbor coupling Ω, in the presence of static disorder of strength W and dephasing of strength γ, and where the last site is coherently coupled to an external environment with sink coupling strength Γ_{trap} and the system is initialized in the first site. For this model, which has been extensively studied in the literature, our analysis allowed us to estimate the critical static disorder above which dephasing can assist transport. Specifically we have seen that W^{cr} varies linearly or inversely with the coupling Γ_{trap} when Γ_{trap} is small or large, respectively.

An essential point of our analysis is the estimate of the optimal dephasing rate in the ballistic regime (and not only in the localized regime as has been done in previous works).

Different regimes have been obtained for the behavior of the optimal dephasing rate γ^{opt}. For W close to W^{cr}, we have $\gamma^{\text{opt}} \sim (W - W^{\text{cr}})/N$, whereas for $\Gamma_{\text{trap}}/\sqrt{N} \ll W \ll \Omega/\sqrt{N}$, the optimal dephasing becomes independent of the coupling to the sink and scales as $\gamma^{\text{opt}} \sim W/\sqrt{N}$. In both the weak- and moderate-disorder regimes, dephasing aids transport even though eigenstates are delocalized and motion is ballistic. This can be explained by the fact that the transfer efficiency is not only determined by the velocity of excitation spreading but also by the time the excitation spends in the site coupled to the sink. Since in the ballistic case the probability to be in the last site experiences large fluctuations, dephasing can help transport by stabilizing the excitation on the exit site and increasing its probability to escape. Finally, for sufficiently strong disorder, $W \gg \Omega/\sqrt{N}$, the quantum states become localized and the optimal dephasing rate becomes N-independent, as has been seen in previous works.

Our main result is that dephasing can help transport even in the ballistic regime in finite systems. Even if our system is too simple to model realistic systems, such as natural light-harvesting complexes, we think that this main result will remain valid in more realistic situations and can help in the design of efficient quantum wires.

ACKNOWLEDGMENTS

Appendix A: Analytical Expression for Transfer Time τ_3 in a 3-site Chain

For a 3-site chain with arbitrary on-site energies ω_i, inter-site hopping Ω, dephasing rate γ, and site 3 coupled to the acceptor system with coupling Γ_{trap}, we may solve Eq. (11) exactly using Wolfram Mathematica to obtain the transfer time

$$\tau_3 = \frac{X_0 + \Omega^2 X_2 + \Omega^4 X_4}{Z}, \tag{A1}$$

where

$$X_0 = \Gamma_{\text{trap}} \left[4 \left(\gamma^2 + (\omega_1 - \omega_3)^2 \right) + 4\gamma\Gamma_{\text{trap}} + \Gamma_{\text{trap}}^2 \right] \tag{A2}$$
$$\times \left[2\gamma \left(3\gamma^2 + \omega_1^2 - 2\omega_1\omega_2 + 3\omega_2^2 - 4\omega_2\omega_3 + 2\omega_3^2 \right) + \Gamma_{\text{trap}} \left(5\gamma^2 + (\omega_1 - \omega_2)^2 \right) + \gamma\Gamma_{\text{trap}}^2 \right],$$

$$X_2 = 48\gamma^2 \left(\gamma^2 + (\omega_1 - \omega_3)^2 \right) + 8\gamma\Gamma_{\text{trap}} \left(15\gamma^2 + (\omega_1 - \omega_3)(5\omega_1 - \omega_2 - 4\omega_3) \right) \tag{A3}$$
$$+ 8\Gamma_{\text{trap}}^2 \left(11\gamma^2 + (\omega_1 - \omega_3)^2 \right) + 24\gamma\Gamma_{\text{trap}}^3 + 2\Gamma_{\text{trap}}^4,$$

$$X_4 = 12 \left(2\gamma + \Gamma_{\text{trap}} \right) \left(4\gamma + \Gamma_{\text{trap}} \right), \tag{A4}$$

$$Z = 2\Omega^2 \Gamma_{\text{trap}} \left(2\gamma + \Gamma_{\text{trap}} \right) \left[2\Omega^2 \left(4\gamma + \Gamma_{\text{trap}} \right) + \gamma \left(2\gamma + \Gamma_{\text{trap}} \right)^2 + 4\gamma(\omega_1 - \omega_3)^2 \right]. \tag{A5}$$

[1] J. M. Moix, M. Khasin, and J. Cao, New J. Phys. **15**, 085010 (2013).
[2] K. D. B. Higgins, S. C. Benjamin, T. M. Stace, G. J. Milburn, B. W. Lovett, and E. M. Gauger, Nature Communications **5**, 4705 (2014).
[3] M. Sarovar and K. B. Whaley, New J. Phys. **15**, 013030 (2013).

[4] J. Grad, G. Hernandez, and S. Mukamel, Phys. Rev. A **37**, 3835 (1988).

[5] F. C. Spano and S. Mukamel, J. Chem. Phys. **91**, 683 (1989).

[6] G. S. Engel, T. R. Calhoun, E. L. Read, T. K. Ahn, T. Mancal, Y. C. Cheng, R. E. Blankenship, and G. R. Fleming, Nature **446**, 782 (2007).

[7] G. Panitchayangkoon, D. Hayes, Kelly A. Fransted, Justin R. Caram, E. Harel, J. Wen, R. E. Blankenship, and G. S. Engel, Proc. Nat. Acad. Sci. USA **107**, 12766 (2010).

[8] M. Sarovar, A. Ishizaki, G. R. Fleming, and K. B. Whaley, Nat. Phys. **6**, 462 (2010).

[9] H. Hossein-Nejad and G. D. Scholes, New J. Phys. **12**, 065045 (2010).

[10] J. Strumpfer, M. Sener, and K. Schulten, J. Phys. Chem. Lett. **3**, 536 (2012).

[11] X. Hu, T. Ritz, A. Damjanovic, and K. Schulten, J. Phys. Chem. B **101**, 3854 (1997); X. Hu, A. Damjanovic, T. Ritz, and K. Schulten, Proc. Natl. Acad. Sci. USA **95**, 5935 (1998).

[12] Y. Zhang, G. L. Celardo, F. Borgonovi, and L. Kaplan, Phys. Rev. E **95**, 022122 (2017).

[13] D. E. Logan and P. G. Wolynes, J. Chem. Phys. **87**, 7199 (1987); D. A. Evensky, R. T. Scalettar, and P. G. Wolynes, J. Phys. Chem. **94**, 1149 (1990).

[14] P. Rebentrost, M. Mohseni, I. Kassal, S. Lloyd, and A. Aspuru-Guzik, New J. Phys. **11**, 033003 (2009); P. Rebentrost, M. Mohseni, and A. Aspuru-Guzik, J. Phys. Chem. B **113**, 9942 (2009).

[15] M. B. Plenio and S. F. Huelga, New J. Phys. **10**, 113019 (2008).

[16] S. Lloyd, M. Mohseni, A. Shabani, and H. Rabitz, arXiv:1111.4982.

[17] G. L. Celardo, F. Borgonovi, M. Merkli, V. I. Tsifrinovich, and G. P. Berman, J. Phys. Chem. C **116**, 22105 (2012); D. Ferrari, G. L. Celardo, G.P. Berman, R. T. Sayre, and F. Borgonovi, J. Phys. Chem. C **118**, 20 (2013).

[18] G. L. Celardo, Giulio G. Giusteri, and Fausto Borgonovi, Phys. Rev. B **90**, 075113 (2014); G. L. Celardo, Paolo Poli, Luca Lussardi, and Fausto Borgonovi, Phys. Rev. B **90**, 085142 (2014).

[19] J. Wu, R. J. Silbey, and J. Cao, Phys. Rev. Lett. **110**, 200402 (2013).

[20] G.G. Giusteri, F. Mattiotti, and G. L. Celardo, Phys. Rev. B **91**, 094301 (2015).

[21] H. Haken and G. Strobl, Z. Physik **262**, 135 (1973).

[22] F. Caruso, A. W. Chin, A. Datta, S. F. Huelga, and M. B. Plenio, J. Chem. Phys. **131**, 105106 (2009).

[23] J. Cao and R. J. Silbey, J. Phys. Chem. A **113**, 13825 (2009).

[24] V. V. Sokolov and V. G. Zelevinsky, Nucl. Phys. **A504**, 562 (1989); Phys. Lett. B **202**, 10 (1988); I. Rotter, Rep. Prog. Phys. **54**, 635 (1991); V. V. Sokolov and V. G. Zelevinsky, Ann. Phys. (N.Y.) **216**, 323 (1992).

[25] G. L. Celardo and L. Kaplan, Phys. Rev. B **79**, 155108 (2009); G. L. Celardo, A. M. Smith, S. Sorathia, V. G. Zelevinsky, R. A. Sen'kov, and L. Kaplan, Phys. Rev. B **82**, 165437 (2010).

[26] F. M. Izrailev, S. Ruffo, and L. Tessieri, J. Phys. A **31**, 5263 (1998).

[27] J. A. Leegwater, J. Phys. Chem. **100**, 14403 (1996).