Upper Limit of Pure Dephasing Time of a Paired-Qubit with Anisotropic Heisenberg Coupling

Jun-ichi Inoue*
National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

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Robustness against noise is essential for qubits used in applications such as quantum computing [1] and sensing [2, 3, 4]. One measure of this property is their relaxation times, which have typically been used in Bloch equations [5, 6, 7]. Systems or materials with longer relaxation times are generally more valued. This tendency is particularly notable in quantum sensing, where operation at room temperature is standard [8]. Consequently, extensive research has been conducted across various fields to achieve longer relaxation times.

The immense importance of long relaxation times in quantum sensing is due to their impact on sensing resolution [8]. Thus, the natural expectation that high-quality samples, such as those with fewer inclusions, defects, and dislocations, are more promising has driven the development of various crystal-growth techniques [9]. However, the situation is not so straightforward, as shown by the counter-intuitive case where intentional phosphorus doping resulted in the longest relaxation time [10].

The pure dephasing time, $\mathsf{T}_2^{[p]}$, which is the main focus of this work, characterizes the dephasing process induced by inhomogeneity that causes the energy levels of qubits to fluctuate [11, 12]. This time is a relevant component of the inhomogeneous transverse relaxation time. The dephasing time typically describes an exponential decay of an in-plane Bloch vector, corresponding to free induction decay (FID). The reason for focusing solely on $\mathsf{T}_2^{[p]}$ in this study is its particular importance in DC-response measurements [8] and the theoretical interest in obtaining its analytical form for a model that is both well-tailored for theoretical studies and experimentally accessible.

*inoue.junichi@nims.go.jp

The essence of pure dephasing time can be captured in a two-level system, i.e., a single spin $1/2$ in a magnetic field with an amplitude that fluctuates according to a Gaussian random process. For later convenience, the result and outline of the derivation using the Lindblad master equation are summarized here [13, 15, 14]. This equation describes the time evolution of the density operator $\rho(t)$ in an open system. For a single two-level system exposed to a pure dephasing or phase-damping process [1], it is $d\rho/dt = -i[\Omega\sigma_z, \rho] + (2L\rho L^\dagger, L^\dagger L\rho - \rho L^\dagger L)/2$, where $\hbar = 1$. In this equation, σ_z is the z component of a usual 2×2 Pauli matrix $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, the constant Ω denotes the energy difference between the two levels, $L = \sqrt{\Gamma_z}\sigma_z$ is the Lindblad operator for the pure dephasing process, and Γ_z characterizes Gaussian noise in the amplitude of the fictitious magnetic field. In this procedure, the pure dephasing time $T_2^{[p]} = 1/(2\Gamma_z)$ is given by one component of an in-plane Bloch vector $\langle\sigma_x(t)\rangle \equiv \mathrm{Tr}[\rho(t)\sigma_x] = \exp[-2\Gamma_z t]\cos(2\Omega t)$. To derive this solution without losing generality, the initial state $\rho(t=0) = (\mathbf{1}+\sigma_x)/2$ was used, corresponding to a state prepared using the $\pi/2$ pulse in usual FID experiments.

In this study, we propose a theoretical and experimentally feasible idea to prolong the pure dephasing time in a qubit system and derive a formula for this time, with NV^- centers in diamond [3, 9, 8, 16] in mind as a test bed. The core idea is to use the interaction between qubits. When an inferior qubit (one with a shorter pure dephasing time) interacts with a superior one, the former benefits and experiences a prolonged dephasing time. Although this scenario seems intuitively plausible, several questions must be addressed to support it: (i) what kinds of interaction would serve, (ii) whether the prolongation has an upper limit, and (iii) how the prolonged dephasing time depends on the interaction. The following sections answer these questions through an analytical expression of the pure dephasing time obtained by solving a Lindblad master equation, which will be introduced shortly. Subsequently, the significance of the findings is also discussed.

Consider two qubits α and β. Each is assumed to connect with its own reservoir, $\mathcal{R}_\alpha$ and $\mathcal{R}_\beta$, respectively. Reservoir $\mathcal{R}_{\alpha(\beta)}$ causes the connected-qubit to dephase at its pure dephasing rate $\Gamma_{\alpha z(\beta z)}$. These qubits are nonequivalent in the sense that unequality of $\Gamma_{\alpha z} > \Gamma_{\beta z}$ is imposed. The two qubits interact with each other in an anisotropic Heisenberg or XXZ manner and their in-plane and longitudinal magnitudes are denoted by $J_{/\!/}$ and J_z, respectively. Schematics of this system are shown in Fig.1. Hereafter, qubit $\alpha(\beta)$ is referred to as the surface (bulk) qubit.

The Lindblad master equation for the total density operator $\rho(t)$ of the

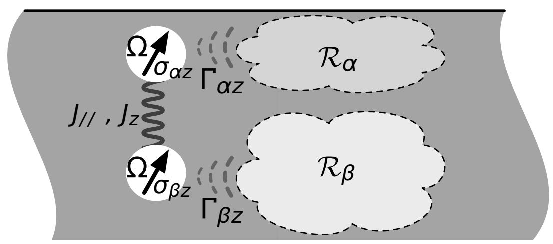

Figure 1: A system considered in this study consists of two qubits, α and β, each of which is described by a Pauli operator $\sigma_{\alpha z(\beta z)}$, respectively. Each connects with its own reservoir $\mathcal{R}_\alpha$ and $\mathcal{R}_\beta$, which induces pure dephasing in the connected-qubit with its rate $\Gamma_{\alpha z} > \Gamma_{\beta z}$. The two qubits interact via anisotropic Heisenberg coupling, $J_{/\!/}$ and J_z. A solid horizontal line indicates a surface of the sample.

two qubits is given by

$$\frac{d\rho(t)}{dt} = -i[H, \rho(t)] + \sum_{\mu=\alpha,\,\beta} \left(L_\mu \rho(t) L_\mu^\dagger - \frac{1}{2} L_\mu^\dagger L_\mu \rho(t) - \frac{1}{2} \rho(t) L_\mu^\dagger L_\mu \right), \tag{1}$$

where the Hamiltonian H is expressed as

$$H = \Omega(\sigma_{\alpha z} \otimes \mathbf{1}_\beta + \mathbf{1}_\alpha \otimes \sigma_{\beta z}) + J_{/\!/}(\sigma_{\alpha x} \otimes \sigma_{\beta x} + \sigma_{\alpha y} \otimes \sigma_{\beta y}) + J_z(\sigma_{\alpha z} \otimes \sigma_{\beta z}), \tag{2}$$

and a set of Lindblad operators $\{L_\mu\}$ describing the independent pure dephasing process is expressed as

$$\{L_{\mu=\alpha,\beta}\} = \left\{ \sqrt{\Gamma_{\alpha z}} \sigma_{\alpha z} \otimes \mathbf{1}_\beta, \quad \sqrt{\Gamma_{\beta z}} \mathbf{1}_\alpha \otimes \sigma_{\beta z} \right\}, \tag{3}$$

with the identity operator $\mathbf{1}_{\alpha(\beta)}$ used for the surface (bulk) qubit. To address questions (i) – (iii), one component of the in-plane Bloch vector for a surface qubit

$$\langle \sigma_{\alpha x}(t) \rangle = \mathrm{Tr}\left[\tilde{\rho}_\alpha(t) \sigma_{\alpha x}\right], \tag{4}$$

is calculated. In this equation, the partial density operator for the surface qubit $\tilde{\rho}_\alpha(t) \equiv \mathrm{Tr}_\beta\left[\rho(t)\right]$ is introduced, where Tr_β denotes the partial trace of the bulk qubit. Assume that $\pi/2$ pulse is injected equivalently into both qubits and we take $\rho(t=0) = (\mathbf{1}_\alpha + \sigma_{\alpha x}) \otimes (\mathbf{1}_\beta + \sigma_{\beta x})/4$, as an initial state without loss of generality.

$$\langle \sigma_{\alpha x}(t) \rangle = e^{-(\Gamma_{\alpha z}+\Gamma_{\beta z})t} \cos(2\Omega t) \times \Bigg[\cos(2J_z t) \cos\Big(\Lambda(J_{/\!/})t\Big) + \frac{2J_{/\!/} \sin(2J_z t) - (\Gamma_{\alpha z} - \Gamma_{\beta z}) \cos(2J_z t)}{\Lambda(J_{/\!/})} \sin\Big(\Lambda(J_{/\!/})t\Big) \Bigg], \tag{5}$$

is obtained after a lengthy, albeit straightforward, calculation, where $\Lambda(J_{/\!/}) \equiv \sqrt{(2J_{/\!/})^2 - (\Gamma_{\alpha z} - \Gamma_{\beta z})^2}$ is defined. To obtain an in-depth understanding of Eq.(5), examinations of three canonical cases, Ising-, XY-, and isotropic Heisenberg-interactions, are helpful.

In case of Ising, we set $J_{/\!/} = 0$ making $\Lambda(J_{/\!/} = 0)$ purely imaginary and it is represented as $\Lambda(J_{/\!/} = 0) = i(\Gamma_{\alpha z} - \Gamma_{\beta z})$ because we assume that $\Gamma_{\alpha z} > \Gamma_{\beta z}$. Using this reduces Eq. (5) to

$$\langle \sigma_{\alpha x}(t) \rangle = e^{-2\Gamma_{\alpha z} t} \cos(2\Omega t) \cos(2J_z t). \tag{6}$$

The decay of $\langle \sigma_{\alpha x}(t) \rangle$ follows a single exponential function with a pure dephasing time $T_2^{[p]} = 1/(2\Gamma_{\alpha z})$. This result is the same as that of the single qubit case. Note that the dephasing time is unrelated to the bulk qubit and their interaction, albeit the two qubits interact. Instead, the effect of J_z appears in the angular frequencies of the oscillation, which are bi-color $2\Omega \pm 2J_z$.

Next, for XY case, substitution of $J_z = 0$ yields Eq. (5) into

$$\langle \sigma_{\alpha x}(t) \rangle = e^{-(\Gamma_{\alpha z}+\Gamma_{\beta z})t} \cos(2\Omega t) \times \left[\cos(\Lambda(J_{/\!/})t) - \frac{\Gamma_{\alpha z} - \Gamma_{\beta z}}{\Lambda(J_{/\!/})} \sin(\Lambda(J_{/\!/})t) \right]. \tag{7}$$

In contrast to the Ising case, the pure dephasing time of $\langle \sigma_{\alpha x}(t) \rangle$ is influenced by the bulk qubit, the manner of which is distinct depending on $J_{/\!/} \lesseqgtr (\Gamma_{\alpha z} - \Gamma_{\beta z})/2 \equiv J_{/\!/c} > 0$.

When $J_{/\!/} > J_{/\!/c}$, $\Lambda(J_{/\!/})$ is real; thus, the time profile of $\langle \sigma_{\alpha x}(t) \rangle$ is considered at its face value, as shown in Eq.(7). The envelope exhibits a single exponential decay with a time constant $1/(\Gamma_{\alpha z} + \Gamma_{\beta z})$, which now depends on the bulk qubit decay rate $\Gamma_{\beta z}$, but not on the interaction strength $J_{/\!/}$. This dephasing rate should be read as $2 \times (\Gamma_{\alpha z} + \Gamma_{\beta z})/2$, which is analogous to the result for a single qubit $2 \times \Gamma_z$. Thus, the surface qubit is thought to effectively acquire a smaller dephasing rate, $(\Gamma_{\alpha z} + \Gamma_{\beta z})/2 < \Gamma_{\alpha z}$, because of XY-interaction with the bulk qubit. This effective value seems reasonable because it is the arithmetic mean of dephasing rates of the two qubits. From this result, we propose that the two qubits for $J_{/\!/} > J_{/\!/c}$ form a similar state to the strongly coupled state in quantum optics [6, 7, 12]. Furthermore, the bulk qubit contributes to the angular frequencies of the oscillations. It is bi-color, similar to the Ising case, but its angular frequencies are now $2\Omega \pm \Lambda(J_{/\!/})$ which depend on $\Gamma_{\beta z}$ and the interaction strength.

For $J_{/\!/} < J_{/\!/c}$, $\Lambda(J_{/\!/})$ is purely imaginary; the envelope of $\langle\sigma_{\alpha x}(t)\rangle$ consists of two exponential decay terms, each of whose rates is $\Gamma_{\alpha z} + \Gamma_{\beta z} \pm \sqrt{(\Gamma_{\alpha z} - \Gamma_{\beta z})^2 - (2J_{/\!/})^2}$, respectively. Among these two rates, the larger one, or the faster decay channel, dominates the overall dephasing characteristics of the surface qubit, so that it is a reasonable pure dephasing rate of $\langle\sigma_{\alpha z}(t)\rangle$ in this study. In contrast to the previous cases, this pure dephasing rate depends on both $\Gamma_{\beta z}$ and $J_{/\!/}$ in a nontrivial manner. Meanwhile, the oscillation is monochromatic, with the intrinsic angular frequency 2Ω. This result is the same as that for a single isolated qubit, although the surface qubit still interacts with the bulk qubit through $J_{/\!/}$.

Finally, in Heisenberg case, $J_{/\!/} = J_z \equiv J_H$, the decay profile of $\langle\sigma_{\alpha x}(t)\rangle$ is immediately found to be the same as that in the XY case for the entire range of J_H because Λ does not include J_z. An explicit form of the pure dephasing rate is obtained by replacing $J_{/\!/}$ with J_H in the XY case. On the other hand, in the oscillation property, one feature is observed: it is a combination of the previous two cases. For $J_H > J_{/\!/c}$, the oscillation is characterized by four angular frequencies $2\Omega \pm 2J_H \pm \Lambda(J_H)$, whereas for $J_H < J_{/\!/c}$, by two angular frequencies $2\Omega \pm 2J_H$, which is similar to the Ising case.

Having examined these three cases, we can now fully characterize our main result for the anisotropic Heisenberg interaction case in Eq. (5). The in-plane Bloch vector of the surface qubit interacting with the bulk qubit exhibits a single or double exponential decay accompanied by multi-colored oscillations. The pure dephasing time $T_2^{[p]}$ can be formulated as follows:

$$\frac{1}{T_2^{[p]}} = \Gamma_{\alpha z} + \Gamma_{\beta z} + \mathrm{Im}\left[\sqrt{(2J_{/\!/})^2 - (\Gamma_{\alpha z} - \Gamma_{\beta z})^2}\right]. \tag{8}$$

By increasing $J_{/\!/}$ from the non-interacting case $J_{/\!/} = 0$, the pure dephasing time of the surface qubit is monotonically prolonged from its bare value $1/(2\Gamma_{\alpha z})$, and finally reaches a maximum of $1/(\Gamma_{\alpha z} + \Gamma_{\beta z})$ at $J_{/\!/c}$, which value is maintained for $J_{/\!/} > J_{/\!/c}$. In addition, J_z does not contribute to the pure dephasing time. On the other hand, the angular frequencies of the oscillation

$2\pi F$ have a parallel form to Eq. (8)

$$2\pi F = 2\Omega \pm 2J_z \pm \mathrm{Re}\left[\sqrt{(2J_{/\!/})^2 - (\Gamma_{\alpha z} - \Gamma_{\beta z})^2}\right]. \tag{9}$$

This multi-colored character of the oscillation also changes qualitatively at $J_{/\!/} = J_{/\!/c}$ from the angular frequencies $2\Omega \pm 2J_z$ to $2\Omega \pm 2J_z \pm \Lambda(J_{/\!/})$. Each of Eqs.(8) and (9) are plotted as a function of $J_{/\!/}/J_{/\!/c}$ in Figs.2 (a) and (b), respectively. It is evident that the signs of $J_{/\!/}$ and J_z are irrelevant as long as $\Gamma_{\alpha z} > \Gamma_{\beta z} > 0$. Thus, the results are valid for both of ferro- and antiferro-magnetic interactions.

These analytical results address the previously raised questions: The pure dephasing time of a qubit with a shorter dephasing time is prolonged through interaction with another qubit with a longer dephasing time. The prolongation increases monotonically but nontrivially with the strength of the interaction between the two qubits. The benefit of the interaction comes solely from the XY component $J_{/\!/}$, and not from the longitudinal component J_z. The prolonged dephasing time eventually saturates at $J_{/\!/} = J_{/\!/c}$, beyond which the time remains constant. The upper limit of pure dephasing time is given by the reciprocal of the reciprocal average of the dephasing times of the two qubits, $T^{[p]}_{\alpha(\beta)2} = 1/(2\Gamma_{\alpha(\beta)z})$. Therefore,

$$T^{[p]}_{\alpha 2} \leq T^{[p]}_{2} \leq \frac{2T^{[p]}_{\alpha 2}T^{[p]}_{\beta 2}}{T^{[p]}_{\alpha 2} + T^{[p]}_{\beta 2}}, \tag{10}$$

as described by Eq.(8). Although the form of the right-hand side or upper limit can be intuitively guessed as it looks familiar, we claim that the novelty of this work is that it explicitly shows how $T^{[p]}_{2}$ depends on $J_{/\!/}$ and $\Gamma_{\alpha z(\beta z)}$ and that $T^{[p]}_{2}$ is free from J_z. This insensitivity to J_z is understandable, because the pure dephasing process of a qubit is caused by the fluctuation of z component of a fictitious magnetic field characterized by $\Gamma_{\alpha z(\beta z)}$, and thus manifests itself in the in-plane motion of the qubit [17]. It is $J_{/\!/}$, not J_z, that influences the in-plane motion. The saturation of the pure dephasing time, whose region is represented in gray in Fig. 2, suggests that the two qubits are considered to form a strongly coupled state. This state could also be monitored in terms of the number of oscillation frequencies. They are doubled from one to two or two to four, depending on $J_z = 0$ or not, respectively, with increasing $J_{/\!/}$ for the given constants $\Gamma_{\alpha z(\beta z)}$.

Now let us consider feasible experimental tests of the results obtained above. A candidate for real systems corresponding to Fig.1 is NV^- centers in

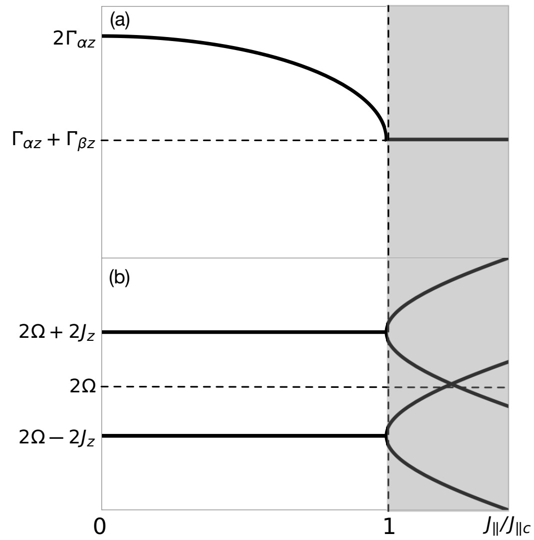

Figure 2: Thick solid lines represent (a) the pure dephasing rate, Eq. (8) and (b) the angular frequencies, Eq. (9), as a function of $J_{/\!/}/J_{/\!/c}$ with fixed constants, $\Gamma_{\alpha z} > \Gamma_{\beta z}$, and J_z. The gray region indicates a strong coupling region. Dashed lines are guides to the eyes.

diamond. The origin of $J_{/\!/}$ in Eq.(8) can be traced back to a magnetic dipole interaction between the surface and bulk qubits [18, 19]. With advancements in fabrication techniques, these centers can now be accurately located and oriented in diamond [20]. Thus, the following experiments would be possible.

Let r be the distance between two qubits. The dipole interaction strength can be simply represented by $J_{/\!/} = J_{/\!/c}(r_c/r)^3$ for $J_{/\!/} < J_{/\!/c}$, with a certain normalization length r_c. The details of r_c, which depend on material characteristics, are beyond the scope of the current study. In this usage, Eq.(8) takes the form

$$\frac{1}{T_2^{[p]}} = \mathrm{Re}\left[\Gamma_{\alpha z} + \Gamma_{\beta z} + (\Gamma_{\alpha z} - \Gamma_{\beta z})\sqrt{1 - \left(\frac{r}{r_c}\right)^{-6}}\right], \tag{11}$$

and is plotted in Fig.3 as a function of r/r_c. The inset shows a double-log plot of $|1/T_2^{[p]} - 2\Gamma_{\alpha z}|$, highlighting power dependence with respect to r in the vicinity of $r/r_c \gtrsim 1$, which is accompanied by the dashed line $\lim_{r\to\infty} |1/T_2^{[p]} - 2\Gamma_{\alpha z}| = (\Gamma_{\alpha z} - \Gamma_{\beta z})\,(r/r_c)^{-6}/2$. Thus, for several samples with different r values but fixed orientations of NV^-s, measurements of pure

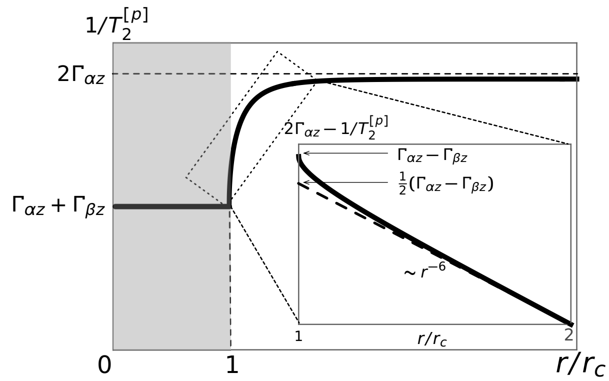

Figure 3: Distance between the two qubits dependence of the pure dephasing rate in a dipole interaction case (main) and double-log plot of $|1/T_2^{[p]} - 2\Gamma_{\alpha z}|$ in the vicinity of $r/r_c \gtrsim 1$ (inset, solid line), with a guide to the eyes $(\Gamma_{\alpha z} - \Gamma_{\beta z})/2 \times (r/r_c)^{-6}$ (inset, dashed line).

dephasing times can test the present theory. In particular, when the pure dephasing time becomes saturated when r is less than a certain value, this suggests a strongly coupled state of the two qubits.

Another test uses the relative orientation of the two qubits while maintaining the distance r. The in-plane interaction strength $J_{/\!/}$ which originates from the dipole interaction, depends on the relative angle θ of the two dipoles as $J_{/\!/} \propto \cos\theta$. In the case of NV^-, the orientation of the dipole vector is considered parallel to the direction from N- to the neighboring vacancy sites. As NV^- has C_{3v} point-group symmetry, where the threefold rotation axis is along the N-V direction, we have finite choices for θ, including the option of ferro- or antiferro-like, although some of them are equivalent. However, considering θ as a continuous variable, we let $J_{/\!/} = J_{/\!/c}\cos\theta$, then Eq.(8) takes the form $1/T_2^{[p]} = \Gamma_{\alpha z} + \Gamma_{\beta z} + (\Gamma_{\alpha z} - \Gamma_{\beta z})\sin\theta$. Hence, when this angle dependence is observed for samples with different θ values and a common r, it further supports this study.

One of the challenges in the application of NV^- centers in diamond for quantum sensing is regarding the locations of the NV^-s. To achieve a finer resolution, a shorter distance between the measured object and the NV^- centers, or in other words, NV^- centers located closer to the diamond surface, is more advantageous. However, this would result in serious damage to the resolution because of the drastically shortened relaxation times of the qubits caused by various types of fluctuations intrinsic to the surface [21]. The concept presented in this paper offers a solution to this problem.

Before concluding the paper, a brief description of previous studies is provided. Studies of an open quantum system with a two-spin have so far assumed mainly semiconductor double quantum dots, whose major interests have been, to name a few, decoherence dynamics, entanglement dynamics, and singlet-triplet conversion rate [22, 23, 24, 25, 26, 27, 28, 29]. In dot systems, two electron spins are considered equivalent and thus treated on an equal footing, which allows the introduction of a sum-operator for the two spins and describes them in terms of singlet and triplet states. Their Hamiltonian has the sum-operator squared, which restricts the interaction of the two spins to an antiferromagnetically isotropic Heisenberg coupling. By contrast, this study naturally introduces an anisotropy into the interaction, $\mathrm{J}_z \neq \mathrm{J}_{/\!/}$ [18, 19], between the two qubits. Until this anisotropy is considered, the important finding that the pure dephasing time is free from the longitudinal component of the interaction is not provided.

A possible extension of the current study is to increase the number of qubits. This interest is inspired by a report that a triple nitrogen-vacancy center in diamond was fabricated by ion implantation [30]. This system would introduce a new "degree of freedom" that a surface qubit is located either at the end or the center of the row. As the number of qubits increases, a semi-infinite length chain of qubits becomes conceivable, aside from feasibility in real systems [32, 33, 34, 31]. The dynamics of a qubit attached to the edge of the chain has been discussed using the Lindblad equation, focusing on non-Hermiticity, specifically exceptional points, $\mathcal{PT}$ symmetry, and the eigenvalues distribution of the Liouville operator in conjunction with the language of topology. Using a chain also allows for the introduction of various kinds of interactions between qubits, such as Su-Schrieffer-Heeger, Kitaev, and others, which are expected to unveil further rich physics.

In conclusion, we propose a theoretical scheme to prolong the pure dephasing time of a qubit by coupling it with another qubit with a longer pure dephasing time. From the analytical solution obtained here, we have shown that there is an upper limit to the time, below which the time is a monotonically but nontrivially increasing function of the in-plane coupling $\mathrm{J}_{/\!/}$ but is insensitive to J_z. This theoretical idea could address the challenges of achieving longer dephasing times for improved sensor resolution. The scheme, presented in a general context, has the potential to be applied to other qubit systems, stimulating further research in those communities.

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