Non-perturbative Dynamical Decoupling Control: A Spin Chain Model

Zhao-Ming Wang\textsuperscript{1,2}, Lian-Ao Wu\textsuperscript{2}, Jun Jing\textsuperscript{3}, Bin Shao\textsuperscript{4}, Ting Yu\textsuperscript{3}

\textsuperscript{1} Department of Physics, Ocean University of China, Qingdao, 266100, China
\textsuperscript{2} Department of Theoretical Physics and History of Science, The Basque Country University (EHU/UPV) and IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain
\textsuperscript{3} Center for Controlled Quantum Systems and Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, New Jersey 07030, USA and
\textsuperscript{4} Key Laboratory of Cluster Science of Ministry of Education, and School of Physics, Beijing Institute of Technology, Beijing 10081, China

This paper considers a spin chain model by numerically solving the exact model to explore the non-perturbative dynamical decoupling regime, where an important issue arises recently\textsuperscript{1}. Our study has revealed a few universal features of non-perturbative dynamical control irrespective of the types of environments and system-environment couplings. We have shown that, for the spin chain model, there is a threshold and a large pulse parameter region where the effective dynamical control can be implemented, in contrast to the perturbative decoupling schemes where the permissible parameters are represented by a point or converge to a very small subset in the large parameter region admitted by our non-perturbative approach. An important implication of the non-perturbative approach is its flexibility in implementing the dynamical control scheme in an experimental setup. Our findings have exhibited several interesting features of the non-perturbative regimes such as the chain-size independence, pulse strength upper-bound, noncontinuous valid parameter regions, etc. Furthermore, we find that our non-perturbative scheme is robust against randomness in model fabrication and time-dependent random noise.

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I. INTRODUCTION

Central to quantum science and technology is to combat decoherence caused by inevitable external noises or quantum operation inaccuracies\textsuperscript{2}. Strategies for controlling a quantum state include the quantum error correction codes\textsuperscript{3–5} and dynamical coupling control such as fast-strong pulses (“bang-bang”) control\textsuperscript{6–12}. One common feature of these dynamical control approaches is that almost all the theories are defined in a perturbative manner. Despite the progress made in theoretical studies and experimental realizations, the perturbation theories still lack a satisfactory understanding of their validity and applicability, especially the divergence issue due to the onset of a possible phase transition. Recently, a careful examination of the dynamical decoupling or bang-bang control has led to new breakthroughs achieved through introducing a non-perturbative dynamical decoupling scheme based on exact stochastic master equations in bosonic baths\textsuperscript{1}. By using this scheme, we showed that there is a threshold and a large pulse parameter region where the effective dynamical control can be implemented, in contrast to the perturbative decoupling schemes where the permissible parameters converge to a point or form a very small subset in the large parameter region admitted by our non-perturbative approach. Our non-perturbative approach has shown impressive flexibility in implementing the dynamical control scheme in experimentation.

This paper uses a spin chain model to explore the non-perturbative dynamical decoupling regime. Our results demonstrate, through new type of environment and new numerical methods, several universal features of the non-perturbative dynamical decoupling emerge. More specifically, we show that there is a threshold and a large pulse parameter region where the effective dynamical control can be implemented.

We model the first spin in an XY-type model as our system of interest and the rest as our environment. The bath spectral density is chosen as a complicated function indicating that the ratios between two arbitrary levels are normally not rational numbers. We have derived an exact “master equation” for our spin system. It should be noted that for the spin environment, the environmental correlation function is very different from that for a bosonic model. However, our results obtained from this particular XY-type model are expected to be applicable to other spin-environment models. Our numerical calculations show that effective control can be made in many different ways either through a multiple pulse sequence, as in the case of bang-bang control, or just a single pulse applied within the bath memory time. The effectiveness of the dynamical control is not sensitive to the size of spin chain, an observation that showcases the universality of our findings. For the spin chain model, we have shown that there is an upper-bound for pulse strength in non-perturbative regimes when the pulse duration is sufficiently large, which is rather counter-intuitive from the point of view of the strong fast pulse control (bang-bang). We also consider the time-independent randomness for coupling constants and site energies of the XY-type spin chain. We show that our results and conclusion are robust to the random couplings and site energies even in...
the strong-coupling limit. Finally, we consider the time-dependent random noise, which may simulate the noisy effects due to additional environmental variables. We show that the quality of dynamical control in the non-perturbative regime is also robust to the influence of the time-dependent noise.

II. THE MODEL

The spin chain model considered here is represented by the following Hamiltonian,

\[ H = H_S + H_B + H_{SB} \]  

where \( H_S \) and \( H_B \) is the system's and environment's Hamiltonian. \( H_{SB} \) is the interaction between the system and environment. We consider an XY-type spin-chain model, where the first spin of the chain is our system of interest and the environment is composed of all the other \( N - 1 \) spins. The system Hamiltonian and control are \( H_S = c(t)Z_1 \), where \( c(t) \) is a time-dependent control function. The control is only applied to the system, and the \( c(t) \) is chosen as a sequence of periodic rectangular pulses:

\[ c(t) = \begin{cases} \Psi & n\tau < t < n\tau + \Delta, n \text{ is integer} \\ 0, & \text{otherwise} \end{cases} \]  

where \( \Psi \) is the pulse strength, \( 1/\tau \) is the pulse frequency and \( \Delta \) is the width of the pulse in one period. The three parameters span the parameter space of the non-perturbative dynamical decoupling scheme as in [1]. The limiting case with \( 1/\tau, \Delta \to 0 \) and \( \Psi \to \infty \) corresponds to the idealized Bang-Bang control.

The XY-type spin-chain Hamiltonian is modeled as

\[ H_{SB} = -J_{1,2}(X_1X_2 + Y_1Y_2), \]  

\[ H_B = - \sum_{i=2}^{N-1} J_{i,i+1}(X_iX_{i+1} + Y_iY_{i+1}) + H_{\text{site}} \]  

where \( J_{i,i+1} \) is the exchange interaction between sites \( i \) and \( i+1 \). The system and environment coupling constant is \( J_{1,2} \). \( X_i, Y_i \) denote the Pauli operators acting on spin \( i \), and \( N \) is the total number of sites. We consider a natural configuration of the spin chain with open ends. The \( z \)-component of the total spin is a conserved quantity implying the conservation of the total excitations in the system. For simplicity, we consider that the system is in the “one-magnon” state, in which the total number of up spins is one and \( J = J_{i,i+1} = 1.0 \). \( H_{\text{site}} \) is the site energy and will be specified in our later discussion. Our numerical calculations show that, within the “one-magnon” subspace, the sign of \( J \) (plus or minus) does not affect the results.

The system dynamics alternates between control and free evolution. We start with a control pulse with the width \( \Delta \), followed by \( \tau - \Delta \) free evolution. The evolution operator of the whole system for the first time interval or period will be \( U_0(\tau - \Delta)U(\Delta) \), where \( U(\Delta) = \exp[-i\Delta H] \) and \( U_0(\tau - \Delta) = \exp[-i(\tau - \Delta)H_0] \). Here \( H_0 \) denotes the free evolution without control. We then repeat the same operations from time \( \tau \) to \( 2\tau \). The bang-bang control theory is the idealized limit, \( \Delta, \tau \to 0 \) and \( \Psi \to \infty \), which has been shown to be able to eliminate the interactions between the system and bath.

We can diagonalize the Hamiltonian \( H \) and \( H_0 \) such that \( H_B = W^\dagger HW, H_{0B} = V^\dagger H_0V \). The evolution operators can therefore be expressed by

\[ U(\Delta) = W \exp[-i\Delta H_B]W^\dagger \]  

\[ U_0(\tau - \Delta) = V \exp[-i(\tau - \Delta)H_{0B}]V^\dagger \]  

Suppose that our system, the first spin, is initially in the state \( |\phi(0)\rangle = |1\rangle \), while the other spins are in the spin down state \( |0\rangle \). The spin chain will be in a product state \( |\Phi(0)\rangle = |1\rangle \otimes |00 \cdots 0\rangle = |100 \cdots 0\rangle \).

After \( m \)-time control, the fidelity at the time \( m\tau \), measuring the survival probability of the initial state \( |\phi(0)\rangle \), can be defined as \( F = \sqrt{\langle \phi(0) | \rho(t) | \phi(0) \rangle} \), where \( \rho(t) \) is the reduced density matrix of the state at the first sites at \( t = m\tau \). The \( N \) eigenvectors and eigenvalues of the Hamiltonian \( H, H_0 \) can be obtained by numerical diagonalization.

In the next section, we will analyzes the quality of dynamical control in terms of the fidelity defined above.

III. RESULTS AND DISCUSSIONS

![FIG. 1: (Color on line) The fidelity after 128-time control pulse \((t = 128\tau)\), the initial state is \(|1\rangle\) at the first spin. The bottom triangular area has no physical meaning since \( \tau \) is always larger than \( \Delta \) by definition. \( \Psi = 8.0, N = 130 \).](image-url)
the spin chain. The periodical rectangle pulses will suppress the disturbing process, a well-known fact in the case of bang-bang control. Fig. plots the contour fidelity as a function of the pulse period \( \tau \) and pulse duration \( \Delta \) at time \( t = 128\tau \) (the \( \Delta - \tau \) phase diagram). It clearly shows that, similar to the dissipative bosonic bath, there is a large parameter region where the dynamical decoupling (or noise suppression) works equally well as shown in the red zone in Fig. The left-bottom corner (\( \Delta \) and \( \tau \to 0 \)) represent the idealized pulses dynamical decoupling, which has the same fidelity as the regimes with parameters \( \tau \) and \( \Delta \) in the red zone. Interestingly, there is an upper-bound for the parameter \( \Delta \approx 1.3 \) in this spin model. The onset of the failure of an effective control is the fundamental restriction of the bath memory time to be discussed later.

![Figure 2](image2)

FIG. 2: (Color on line) The fidelity as a function of number of sites \( N \) under free and control Hamiltonian, where \( \Psi = 8.0, \Delta = 1.2, \tau = 1.3 \) and \( t = 128\tau \).

The analysis presented above is for the case when the number of sites, \( N=130 \). Since our environment contains a finite number of spins, it is important to analyze the length dependence of our control scheme, in order to eliminate the finite size effects. In Fig. we plot the fidelity of the system state at the time \( t = 128\tau \) for varied chain lengths or the numbers of sites. We compare the fidelity of free evolution with the case that the dynamical control is applied in this figure. The horizontal axes represents the number of sites \( N \) and the vertical is the fidelity. There are several interesting new features in this figure. First, for the free evolution, while fidelity is not good as expected, clearly the fidelity shows significant oscillation for odd-even numbers of sites, whose magnitude decreases with \( N \). This is a typical finite-size effect. However, the quality of the non-perturbative dynamical decoupling, in the non-perturbative control pulse region with \( \Delta = 1.2, \tau = 1.3 \), does not depend on the chain length \( N \), as shown clearly in the figure. The fidelity is close to 0.98 for all the total numbers of spins \( N \). This implies that the finite size effect of the chain, dose not affect our results and conclusions.

![Figure 3](image3)

FIG. 3: (Color on line) The fidelity as a function of control times \( t \). \( \Psi = 8.0, \Delta = 1.2, \tau = 1.3, N = 130 \). We explain these curves in the text.

The above analysis is for the case with a fixed time \( t = 128\tau \). Now we discuss the time evolution of the fidelity. Fig. plots the fidelity versus time \( t \). We compare the five cases: free evolution, and controlled evolution under the one of the following four conditions: (1) constant coupling \( J \), (2) band broadening, (3) randomness coupling \( J + \gamma \text{rand}(i) \) and (4) stochastic coupling \( J + \eta \text{rand}(i) \). Here the band broadening refers to the uncorrelated random potentials, which is defined by \( H_{\text{site}} = \epsilon \sum \text{rand}(i) \) (\( \epsilon = 0.5 \) in the figure) and generated in the process of physical fabrication. \( \gamma \text{rand}(i) \) is a random function of sites \( i \), where \( \gamma \) (taken as 0.5 in the figure) is the magnitude of the random function. \( \text{rand}(i) \) denotes a stochastic number uniformly distributed in the interval \((-1, 1)\). It is noticeable that the dynamical control quality, characterized by the fidelity, does not change significantly with these two types of random distributions, even in the long-time limit, which indicates that our non-perturbative dynamical decoupling control is robust against the defect or frustration in experimental fabrication of the spin systems. Once the spin-chain is generated, it does not change with time. However, it is important to consider a time-dependent random noise due to an external agent (or environment). Equally interesting, our numerical scheme allows us to model the noise as the perturbation by \( \eta \text{rand}(i) \) (\( \eta = 0.1 \) in Fig. , which changes randomly before each pulse period, i.e. the random number \( \eta \text{rand}(i) \) is constant within one period but varies for different periods. Surprisingly, the control quality is shown to be robust compared to the cases without the time-dependent noises, as shown by the inset of Fig. . Again, our analysis shows that another universal features of our finding based on the non-perturbative dynamical decoupling scheme.

In Fig. we plot the contour fidelity as a function of pulse strength \( \Psi \) and \( \tau/\Delta \) for given \( \Delta = 0.1, 0.5, 1.2 \), re-
and an upper-bound for the strength in non-perturbative regimes. There is always a region where the dynamical control works with high fidelity, as shown in the red zone where $F > 0.95$. Surprisingly, there are a lower-bound and an upper-bound for the strength in non-perturbative regimes. For instance, when $\Delta = 0.5$, this region is $6.0 < \Psi < 9.0$ when $1.0 < \tau/\Delta < 1.6$. When the parameter is close to the bang-bang regime, e.g., $\Delta = 0.1$, there is only a lower-bound. In other words, only bang-bang requires strong pulse strength, while non-perturbative control does not.

### IV. ENVIRONMENT CORRELATION BY FESHBACK PROJECTION-OPERATOR PARTITIONING TECHNIQUE

Using $PQ$ partitioning technique [1], an $n$-dimensional wave function $\psi_t$ can be divided into two parts: an interested one-dimensional vector $P(t)$ and the rest $(n - 1)$-dimensional vector $Q(t)$. $\psi_t, H_{eff}$ can be simply written as

$$
\psi_t = \begin{bmatrix} P \\ Q \end{bmatrix}, \quad H_{eff} = \begin{bmatrix} h & R \\ R^T & D \end{bmatrix}
$$

where the $1 \times 1$ matrix $h$ and $(n - 1) \times (n - 1)$ matrix $D$ are the self-Hamiltonian living in the subspaces of $P$ and $Q$. For our model, $h$ is the control function $c(t)$ and $R = [J \ 0 \ 0 \ ... \ 0]$ is $1 \times (n - 1)$-dimensional.

$$
D = \begin{bmatrix} 0 & J & .. & 0 & 0 \\ J & 0 & .. & 0 & 0 \\ .. & .. & .. & .. & .. \\ 0 & 0 & .. & 0 & J \\ 0 & 0 & .. & J & 0 \end{bmatrix}
$$

In the selected one dimensional subspace, $P$ satisfies

$$
i\dot{P} = hP - i \int_0^t dsg(t,s)P(s)
$$

where in our case $g(t,s) = g(t - s) = Re^{-iD(t-s)R^T}$, $\Re e^{-iD(t-s)L^T}$, $D$ is the diagonalized matrix, $D = L^TDL$. Specifically,

$$
g(t-s) = J^2 \sum |L_{1k}|^2 e^{-iE_k(t-s)}
$$

where $L_{1k}$ are matrix elements of the first row and the $k$th column of the matrix $L$ and $E_k$ is the $k$th eigenvalues of $D$.

In general, Eq. (9) is a one-dimensional exact equation [13] for arbitrary baths and has to be numerically solved. However, $g(t,s)$, is often reduced to $g(t - s)$, is a bath correlation function and often has common behaviors that hardly depend on the details of baths. Normally, the real part of the function $g(t - s)$ starts from one and decays (rapidly) to zero with time $t - s$, unless baths have limited numbers of frequencies, for instance, the spectral distribution of a few Harmonic oscillators. The imaginary part corresponds to an oscillating factor and is not responsible for the leakage from the $P$ space, resulting in the renormalized energies. Fig. 4 shows the behaviors of the real part of the environment correlation function of this specific model. The spectrum structure of $D$ in our model is sufficiently complicated such as the ratios of any two energy levels are not rational numbers.
We see that the correlation function (memory function) vanishes at the lifetime $\tau \approx 1.7$, with a few small damping oscillations due to the finite number of spins. Fig. 5 also shows that the effect of randomness on the correlation function ($\gamma_{\text{rand}}(i)$) of $J$ (See the four dashed lines). The randomness only affects the correlation function after lifetime and different kinds of randomness yield the out-of-phase curves, meaning that the randomness may eliminate the possibility of the revival of the memory after the lifetime. Strong and fast pulses suppress the decay rate and effectively prolong the lifetime of the correlation function. This is one important mechanism underlying the dynamical decoupling control (see, e.g., [12] and references therein). On the contrary, our valid parameter region may allow very wide and slow pulses, e.g. $\tau \approx 1.3$ (almost the lifetime), which is obviously beyond the known perturbative suppression mechanism. Our calculations confirm further that the valid parameter $\tau$ should be chosen within the lifetime. That is, the dynamical control is effective when the environment is still in non-Markovian regimes.

V. CONCLUSIONS

In conclusion, we have investigated a non-perturbative approach to dynamical control theory through an XY-type spin model. We have shown that dynamical control with high fidelity can be achieved in a large control parameter region. There are many interesting features arising from this spin-chain model including the chain-size independence, the pulse strength upper-bound, non-continuous valid parameter regions, etc.

Our initiative has opened the new avenue for exploring the dynamical decoupling scheme in a more realistic situation allowing non-idealized pulses. Our results suggest that the non-perturbative approach may be applicable to various physical systems such as the liquid state NMR with a small number of spins [14][16], solid-state NMR [17][18], optical lattices [19], or quantum dots [20].

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