Dynamical protection of nonclassical correlation in a quantum algorithm

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A quantum memory interacts with its environment and loses information via decoherence as well as incoherence. A robust quantum control that prepares, preserves, and manipulates nonclassical correlations even in the presence of environmental influence is of paramount importance in quantum information processing. A well-known technique to suppress decoherence, namely Dynamical Decoupling (DD), consists of a sequence of rapid flips applied to the system in order to refocus the system-environment interactions. In this work, we integrate DD with quantum gates using optimal control techniques to realize robust quantum gates which offer protection against decoherence. To investigate the protection of non-classical correlation, we study the evolution of quantum discord in Grover’s search algorithm implemented with dynamically protected gates. Using a two-qubit NMR system, we experimentally demonstrate a significant protection against decoherence and incoherence. We find better performances by phase alternating DD sequences with suitable spacings between the DD pulses. Interestingly, we also find that DD sequences based on $\pi/2$ pulses perform as well as or even better than those with $\pi$ pulses in protecting the non-classical correlation. We also support the experimental results by analyzing the robustness of various DD schemes.

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I. INTRODUCTION

Quantum information processing (QIP) often provides classically inaccessible shortcuts to computational problems. Quantum correlations such as quantum discord (QD) and quantum entanglement are regarded as precious resources for QIP [1–3]. In this sense, it is important to preserve these resources during the process of computation. A quantum register interacts with its environment and suffers loss of information stored in it via decoherence. In practice, another important source of information loss is via incoherence, which results from the spatial inhomogeneity in the control fields [4]. Therefore it is necessary to realize noise-free quantum controls which preserve quantum correlations. Dynamical decoupling (DD) involves modulating the system-environment interaction and thereby suppress decoherence as well as incoherence [5, 6]. It usually consists of a sparse sequence of instantaneous qubit-flips to systematically modulate the system-environment interaction. Unlike the fault-tolerant schemes based on error-correction or decoherence-free subspaces, DD requires no additional resource in terms of ancillary registers [7–9]. Accordingly, DD has been widely studied and implemented experimentally [10–13]. Recently several experimental studies have been performed towards protecting quantum correlations in quantum memory [14, 15]. More recently, combining DD and quantum gates has also been studied theoretically [16] as well as experimentally [17–19].

In this work, we incorporate DD within the optimal control procedure, which not only avoids the manual slicing of the gate segments, but also naturally takes care of DD pulse-errors. Moreover, this procedure alleviates the need for the explicit inclusion of system-environment interactions and therefore strengthens the closed-quantum system approximation used in the standard optimization protocols. In particular, we demonstrate realizing protected gates by combining DD and Gradient Ascent Pulse Engineering (GRAPE) protocol [20]. As a specific case, we study the efficiency of various DD schemes in preserving QD in Grover’s search algorithm.

In sections II and III, we provide brief theoretical descriptions of DD-protected gates and QD respectively. We shall describe the results of NMR experiments and numerical simulations in section IV. Finally we conclude in section V.

II. DYNAMICALLY PROTECTED GATES

We consider a homonuclear pair of spin-1/2 nuclei forming a two-qubit liquid-state NMR system. The rotating-frame Hamiltonian of the system is

$$H_S = -\omega_1 I_{1z} - \omega_2 I_{2z} + 2\pi J I_{1z} I_{2z},$$

(1)

where $\omega_i$ are resonance off-sets, $J$ is the indirect spin-spin coupling constant, and $I_{iz}$ are the $z$-components of the spin-angular momentum operators. In this frame, we also consider a control Hamiltonian,

$$H_C(t) = \Omega_x(t)(I_{1x} + I_{2x}) + \Omega_y(t)(I_{1y} + I_{2y}),$$

(2)

where $\Omega_x(t)$ and $\Omega_y(t)$ represent the $x$ and $y$ components of the amplitude and phase modulated RF field. Simultaneously, we also consider the system-environment

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interaction Hamiltonian $H_{SE}(t)$, so that the total Hamiltonian is of the form

$$H(t) = H_S + H_C(t) + H_{SE}(t).$$  

(3)

While the system-environment interaction Hamiltonian $H_{SE}$ that is responsible for the decoherence, is usually hard to characterize, it is still possible to modulate it using a sequence of instantaneous spin-flips. The goal here is to achieve a quantum operation while protecting the quantum register against environmental decoherence. In the following, we describe a simple procedure for integrating DD with QC to achieve a protected quantum operation.

Suppose a quantum operation is realized by the control fields $\{\Omega_x(t),\Omega_y(t)\}$. In practice, time-discretized amplitudes are used, i.e., $\Omega_x(t) = \Omega_x(t,k)$ during $t \in [(k-1)\Delta t,k\Delta t]$, such that the control parameters are piecewise constant amplitudes $\{\Omega_{x,k},\Omega_{y,k}\}$ (see Fig. 1). The ideal closed-system unitary for the $k$th segment is

$$u_k = \exp[-i(H_S + H_{C,k})\Delta t],$$  

(4)

where

$$H_{C,k} = \Omega_{x,k}(I_{1x} + I_{2x}) + \Omega_{y,k}(I_{1y} + I_{2y}),$$  

(5)

and $\Delta t$ is the segment duration.

In the presence of environmental interaction however, the actual open-system propagator for the $k$-th segment becomes

$$u_k^{op} = \exp[-i(H_S + H_{C,k} + H_{SE})\Delta t],$$  

(6)

which acts on the joint system-environment state. Subsequent tracing out of the environmental part results in decoherence of the quantum system. DD pulses interrupt the system-environment evolution and thereby suppress decoherence.

Let $P_j = \exp(-i\beta I_{\alpha_j})$ be the $j$th DD propagator ($j \in [1,M]$) sandwiched between the effective unitaries $U_j$ and $U_{j+1}$ (see Fig. 1). In this work, we study DD sequences with phases $\alpha_j \in \{x,y\}$ and DD flip-angles $\beta = \pi/2$ (as in WAHUHA [21, 22]) and solid echo [23, 24]), as well as $\beta = \pi$ (as in CPMG [25, 26], XY-4 [27, 28]).

The overall propagator for the protected sequence is

$$U_P = U_{M+1} \prod_{j=1}^M P_j U_j.$$  

(7)

Using the toggling-frame picture [19, 24], we may rewrite the above in the form,

$$U_P = U_{M+1} \prod_{j=1}^M \tilde{U}_j,$$  

(8)

where the toggling frame unitaries $\tilde{U}_j = T_j^U U_j T_j$, and $T_j = P_{j-1} T_{j-2} \cdots P_1$ and $T_1 = T_{M+1} = 1$. Given a target propagator $U_T$, we optimize the control amplitudes

$$\Omega_{\text{max}}^x, \Omega_{\text{max}}^y$$

which maximize the fidelity

$$F(U_P,U_T) = \text{Tr} \left[ U_P^\dagger U_T \right] / \text{Tr} \left[ U_T^\dagger U_T \right].$$  

(9)

Unlike the previous works on the protected gates [18, 19], here we integrate periodic, full-amplitude, DD pulses in the optimal control procedure itself, by pre-assigning segments and freezing their amplitudes and phases. The main advantage of this method is that the imperfections in the DD pulses, like RF inhomogeneity, are also accounted and corrected by the remaining segments. Moreover, there is no need for the manual slicing of control pulses to incorporate DD pulses.

Before we discuss the experimental and numerical studies, we first briefly review quantum discord and its evolution during different stages of Grover’s algorithm.

### III. QUANTUM DISCORD (QD)

Quantum entanglement is considered as an important resource in QIP [29, 30]. Even when the entanglement is absent, a bipartite quantum system $(S,A)$ may possess another useful type of quantum correlation known as quantum discord (QD) [31]. QD is quantified by the minimal mismatch between the mutual information obtained in two classically equivalent, but quantum mechanically distinct ways. As can be seen from Fig. 2, the mutual information can be expressed either as

$$I(S : A) = H(A) + H(S) - H(S,A),$$  

(10)

or as

$$J(S : A) = H(S) - H(S|A).$$  

(11)

In classical information,

$$H(X) = - \sum_x p_x \log_2 p_x$$  

(12)
FIG. 2. Venn diagram representing the total information $H(S, A)$ of a bipartite system. $H(A)$ and $H(S)$ are individual information of the system $A$ and $S$ respectively, $I(S : A)$ is the mutual information and $H(S|A)$ and $H(A|S)$ are conditional entropies.

is the Shannon entropy obtained using the probabilities $p_x$ of $x$th outcome. Similarly, the joint entropy

$$H(S, A) = - \sum_{a, s} p(s, a) \log_2 p(s, a), \quad (13)$$

is obtained using the joint probabilities $p(s, a)$ and the conditional entropy

$$H(S|A) = - \sum_{a, s} p_a p(s|a) \log_2 p(s|a), \quad (14)$$

is obtained using the conditional probability $p(s|a)$, which is the probability of occurrence of outcome $s$ given that the outcome $a$ has occurred.

In quantum information, we replace the Shannon entropy with von Neumann entropy, i.e.,

$$H(\rho_X) = - \sum_x \lambda_x \log_2 (\lambda_x), \quad (15)$$

where $\lambda_x$ are the eigenvalues of the density matrix $\rho_X$. The joint von Neumann entropy $H(S, A)$ is evaluated using the eigenvalues $\lambda_{s,a}$ of the full density matrix $\rho_{S,A}$. On the other hand, the conditional entropy $H_n(S|A)$ is evaluated using the eigenvalues $\lambda_{s|a,n}$ of the post-measurement density matrix $\rho_{S|A_n}$ after carrying out a measurement along a basis $\{\Pi^2\}$.

QD is defined as,

$$D(S|A) = I(S : A) - \max_{\Pi} J(S : A) \quad (16)$$

where $J(S : A)$ is maximized over all the possible orthonormal measurement bases [31, 32]. Since QD is also regarded as an important resource for quantum computing, it is necessary to understand its evolution during quantum algorithms. In the following we discuss the evolution of QD in Grover’s search algorithm.

**QD in Grover’s algorithm**

Grover’s algorithm identifies a marked item in an unsorted database of $N$ items in $O(\sqrt{N})$ iterations, while a classical algorithm needs $O(N)$ iterations on an average. The algorithm starts with initializing a quantum register into an uniform superposition

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k\rangle. \quad (17)$$

It then uses an oracle

$$U_W = \sum_{k=0}^{N-1} (-1)^{\delta_{k, k_0}} |k\rangle\langle k| \quad (18)$$

that flips a marked state $|k_0\rangle$, and a diffusion operator

$$U_D = 2|\psi_0\rangle\langle \psi_0| - 1, \quad (19)$$

which inverts each of the basis states about the mean. Together these two operators constitute a Grover’s iterate, i.e., $U_G = U_D U_W$, that amplifies the marked state amplitude.

The top trace of Fig. 3 displays various stages in the Grover’s algorithm up to six iterations. The middle trace shows the periodic evolution of the probability $\langle k_0 | k_0 \rangle$ of the marked state $|k_0\rangle = |01\rangle$. The bottom trace shows the corresponding evolution of QD over six iterations. As expected, QD vanishes whenever the system reaches the marked state - which is a classical state. QD vanishes also for uncorrelated states of the form $\rho_S \otimes \rho_A$ not involving mutual interaction between $S$ and $A$. The question that we ask is, how does QD evolve in a noisy channel implementing Grover’s algorithm, and how well it can be protected by interleaving the Grover’s iterate
with DD. In the following section, we explore the answer to the above question by NMR based experiments.

IV. EXPERIMENTS

In our NMR experiments we utilize the two spin-1/2 proton nuclei of Cytosine dissolved in deuterated dimethylsulfoxide (DMSO-D$_6$). All the experiments are carried out on a Bruker 500 MHz NMR spectrometer at an ambient temperature of 300 K. The resonance offsets of the two protons are 436 Hz and −436 Hz, while the scalar coupling constant $J = 7.0$ Hz. Starting from the thermal equilibrium state $I_{Sz} + I_{Az}$, we use the spatial averaging technique [33] to prepare the pseudopure state (PPS) $(1 - \epsilon) I/4 + \epsilon|00\rangle\langle00|$, where $\epsilon \sim 10^{-5}$ is the purity factor typically present in NMR systems.

We generated the DD-protected oracle operator $U_W$ corresponding to the marked state $|k_0\rangle = |01\rangle$ and the diffusion operator $U_D$ by incorporating DD pulses into the GRAPE optimal control technique [20, 34] as described in section II. To investigate the dependence on the spacing between DD pulses, we generated two sets of protected gates with spacings of 1000 and 2000 GRAPE segments. Each GRAPE segment was of duration 5.1 $\mu$s. The fidelities of these GRAPE pulses, each about 75 ms long, were above 0.99 after averaging over 10% RF inhomogeneity distribution.

To estimate QD, we need to obtain the density matrix at various stages of Grover’s algorithm (see Fig. 3). The density matrix is generally obtained using quantum state tomography (QST) which involves a set of independent experiments (on identically prepared states) each measuring a particular set of observables. The expectation values are then obtained by measuring the signal intensities. We have adopted a QST procedure that results in only absorptive spectral lines which precisely quantify the expectation values without requiring any further numerical processing.

After obtaining the experimental density matrix $\rho_{\text{exp}}$,
we estimated QD via the optimal set of measurement bases proposed by Lu et al. [32]. Similarly, we also estimated the probability \( \langle k_0 \rangle = \langle k_0 | \rho_{\text{exp}} | k_0 \rangle \) of the marked state for \( |k_0\rangle = |01\rangle \). Fig. 4 (a) displays experimentally estimated QD values (in units of \( r^2 / \log_2 2 \)) at various stages of the Grover’s algorithm for up to six iterations, with unprotected (bottom trace) as well as various DD-protected Grover’s iterates. Fig. 4 (b) displays the corresponding probability of the marked state \( |01\rangle \). In all the cases, we observed that the experimental values are in good agreement with the idealized predictions represented by solid lines (also described in Fig. 3). The lower contrast between the theoretical prediction and experimental values indicate high-quality of quantum controls as well as low inherent noise in the NMR system.

To further investigate the power of DD protection, we deliberately introduced incoherence in the form of linear static-field inhomogeneity along the z-axis by using approximately 5 mG/cm pulsed-field-gradient (PFG). It introduces roughly about two to three radians of phase distribution for \( 10^5 \) segments of the GRAPE sequence, over the volume of the sample. The total duration for six Grover-iterations was about 0.9 second, and the translational diffusion of the molecules over this period further introduces randomness in the overall dephasing. The bottom trace of Fig. 4 (c) displays the experimentally measured QD values with unprotected Grover iterate in the presence of such an incoherence. Clearly, the QD profile without DD protection shows little correlation with the ideal QD trajectory. The other traces of Fig. 4 (c) display the experimental QD values under various DD-schemes as indicated. The best protection was achieved by the DD sequence consisting of \( \pi / 2 \) pulses with alternating \( x \) and \( y \) phases separated by 1000 GRAPE segments.

We now try to extract some general features from the experimental data. Fig. 5 shows the average root-mean-square (RMS) deviation between the experimental and idealized theoretical values displayed in Fig. 4 for various DD parameters. While we do not see much contrast between the various DD-protection schemes in the natural NMR conditions (without additional incoherence; left-column of Fig. 5), the DD-protection under additional incoherence leads to some interesting observations (right-column of Fig. 5). First of all, generally the protected gates with various DD parameters showed significant reduction in the RMS deviation of QD as well as probability in the presence of incoherence (right column of Fig. 5). Secondly, the protection with alternating \( x \) and \( y \) phases (top trace of Fig. 5) appear to show superior performance than with constant phase. Similar observations made by previous reports indicate that DD with alternating \( x \) and \( y \) pulses are more robust against pulse imperfections than with constant phase [7]. It has also been shown that a DD sequence with a constant phase eliminates the component of system-environment (SE) interaction which is orthogonal to the DD-phase, whereas a DD with alternating \( x \) and \( y \) phases help focusing all components of SE interactions [12]. Thirdly, the spacing between the DD flips is also crucial. In our experiments, the DD-pulses in the middle of every 1000 GRAPE segments performed much better than that of 2000 segments. This aspect of DD protection had been studied earlier [11, 35]. Finally and most interestingly, the DD flip-angles of \( \pi / 2 \) outperformed that of \( \pi \). The \( \pi / 2 \) DD-schemes modulate the system-environment interactions in similar ways as in WAHUHA [36] and solid-echo sequences [24], and thereby suppress decoherence. To investigate these aspects further, we carried out numerical simulations as described below.

**Numerical simulations**

We now describe numerical simulations to understand the relative performances of various DD-protected Grover iterates \( U_{PG} \) in terms of their robustness against important practical errors. We mainly focus on (i) the flip-angle error and (ii) an uniform phase-error for each GRAPE segment including the DD-pulse. In practice, the former is predominantly due to mis-calibration of RF-amplitudes or errors in resonance offsets, while the latter might arise due to the dielectric properties of the sample. All the GRAPE pulses corresponding to the Grover iterate \( U_{PG} \) with various DD-protections were subjected to either of the above pulse errors, and we estimated the mean fidelities over six-iterations \( F = \)
Phase alternation

No DD x x/y

Mean fidelity

Without incoherence

Phase alternation

No DD x x/y

Mean fidelity

With incoherence

Phase alternation

No DD x x/y

Mean fidelity

Segments between DD

Without incoherence

Mean fidelity

Segments between DD

With incoherence

Mean fidelity

FIG. 6. Mean fidelity up to six Grover iterates $F = \frac{1}{n} \sum_{i=1}^{n} F(U_{PG}^{j}, U_{G}^{j})$ with flip-angle error (filled bars) and with phase error (empty bars) for various DD protection parameters in the absence (left column) and in the presence of incoherence (right column).

$\frac{1}{n} \sum_{i=1}^{n} F(U_{PG}^{j}, U_{G}^{j})$ (see Eq. 9) averaged over the pulse errors. The results corresponding to flip-angle and phase errors are shown by solid and empty bars respectively in the left column of Fig. 6. To understand the robustness in the presence of incoherent noise, we calculated the mean fidelities $\bar{F}$ by averaging over an incoherent field ranging from $-10$ Hz to $+10$ Hz. The corresponding results are shown in the right column of Fig. 6. It is clear that the unprotected Grover iterate is most sensitive to the incoherent noise and loses fidelity drastically, which explains the poor results of QD and probability of the marked states in the bottom traces of Fig. 4. However, the Grover iterates protected by $\pi/2$ pulses with alternating $x$ and $y$ phases with a spacing of 1000 GRAPE segments showed the best performance as was also observed in the experiments (see Figs. 4 and 5). Thus we deduce that although various DD-protected schemes considered here are comparable in the absence of incoherence, certain DD-protectors are more robust against incoherence and hence are superior in preserving the quantum correlations.

V. CONCLUSIONS

Quantum correlations such as quantum discord and quantum entanglement form the resource that fuels the quantum information processors. In this work, we experimentally studied the evolution of quantum discord as well as the probability of a marked state over six iterations of Grover’s quantum search algorithm on an ensemble of spin-1/2 nuclear pairs using nuclear magnetic resonance methods. Unlike the earlier works, we have integrated the dynamical protection into GRAPE optimal control protocol by pre-assigning the positions of dynamical flips. In this way, protected quantum gates are robust by construction against the external noise. Similar protocol can also be incorporated in other optimal control techniques such as Bang-Bang [37], Krotov [38], etc. We also studied various dynamically protected Grover’s iterations experimentally. While the protected gates performed generally better, to investigate the extent of protection, we introduced an additional incoherent noise in the form of a pulsed field gradient. In this case, we observed a significant benefit of dynamically protected gates. However, we found that phase alternating schemes with appropriate spacing of dynamical flips lead to the best protection against the external noise. Interestingly, we also found that the dynamical protection with $\pi/2$ flip-angles are comparable to or even outperforming those with $\pi$. We have supported our experimental findings with numerical simulations. We believe that this study will be useful in understanding dynamical protections and thereby designing robust quantum controls.

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