Quantum Simulation of Dzyaloshinsky-Moriya Interaction

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Quantum simulation of a Hamiltonian \( H \) requires unitary operator decomposition (UOD) of its evolution operator, \( (U = \exp(-iHt)) \) in terms of experimentally preferable unitaries. Here, using Genetic Algorithm optimization, we numerically evaluate the most generic UOD for the Hamiltonian, DM interaction in the presence of Heisenberg XY interaction, \( H_{DH} \). Using these decompositions, we studied the entanglement dynamics of Bell state in the Hamiltonian \( H_{DH} \) and verified the entanglement preservation procedure by Hou et al. [Annals of Physics, 327 292 (2012)].

I. INTRODUCTION

Algorithms with exponential speedups over classical counterparts [11, 2], simulation of quantum systems [3, 4] and testing basic principles of quantum mechanics [6, 7] makes quantum Information processing (QIP) and quantum chemistry and draws attention recently by solving problems like – molecular Hydrogen simulation [4], calculations of thermal rate constants of chemical reactions [5] and quantum chemical dynamics [9].

Dzyaloshinsky-Moriya (DM) interaction is an anisotropic antisymmetric exchange interaction arising from spin-orbit coupling [10, 11]. It was proposed by Dzyaloshinski to explain the weak ferromagnetism of antiferromagnetic crystals (\( \alpha-Fe_2O_3, MnCO_3 \)) [10]. DM interaction is crucial in the description of many antiferromagnetic systems [12–14] and is important in the entanglement properties of the system. Here we present a generic unitary operator decomposition which will help to simulate the Hamiltonian – DM interaction in the presence of Heisenberg XY interaction – in a two qubit system with almost any basic interaction between them.

Long-lasting coherence and high fidelity controls in nuclear magnetic resonance (NMR) are ideal for quantum information processing. Experimental implementation quantum algorithms (Deutsch-Jozsa algorithm, Grover’s search algorithm and Shor’s algorithm of factorization), testing basic principles of quantum mechanics (nohiding theorem [6] and Leggett-Garg inequality [7]) and quantum simulation (hydrogen molecule [4] and system with competing two and three Body interactions [15]) were performed in Liquid state NMR (LSNMR).

Genetic algorithms (GA) are stochastic global search method based on the mechanics of natural biological evolution [16]. It was first proposed by John Holland in 1975 [17]. GA operates on a population of solutions of a specific problem by encoding the solutions to a simple chromosome-like data structure, and applies recombinant operators. GAs are attractive in engineering design and applications because they are easy to use and are likely to find the globally best design or solution, which is superior to other design or solution [18]. Here we used Genetic algorithm optimization for solving UOD for generic DM Hamiltonian with Heisenberg-XY interaction.

Section II deals with theoretical discussion of DM Hamiltonian simulation followed by experimental implementation in Section III.

II. THEORY

DM interaction in the presence of Heisenberg XY interaction \( H(J, D) \) is,

\[
H(J, D) = J (\sigma_1 \sigma_2 + \sigma_1 \sigma_2) + D (\sigma_1 \sigma_2 - \sigma_1 \sigma_2), \tag{1}
\]

where \( J \) and \( D \) respectively represents the strength of Heisenberg and DM interactions.

Experimental simulation of \( H(J, D) \) (Eqn. 1) in a quantum system (with Hamiltonian \( H_{sys} \)) requires UOD of evolution operator \( U(J, D, t) \),

\[
U(J, D, t) = \exp(-iH(J, D) \times t), \tag{2}
\]

in terms of Single Qubit Rotations \( R^a(\theta, \phi) \) (\( \theta \) angle rotation along \( \phi \) axis on \( n^{th} \) spin),

\[
R^a(\theta, \phi) = \exp(-i\theta/2 \times [\cos \phi \sigma_n + \sin \phi \sigma_n]), \tag{3}
\]

and evolution under system Hamiltonian \( U_{sys} \) (Eqn. 4),

\[
U_{sys}(t) = \exp(-iH_{sys} \times t). \tag{4}
\]

Without losing generality, Eqn. 2 can be written as,

\[
U(\gamma, \tau) = \exp(-i[(\sigma_1 \sigma_2 + \sigma_1 \sigma_2) + \gamma (\sigma_1 \sigma_2 - \sigma_1 \sigma_2)] \times t), \tag{5}
\]

where \( \gamma \) represents the relative ratio of interaction strengths (\( \gamma = D/J \)) and \( \tau = J \times t \).

Eqn. 5 forms the complete unitary operator for the Hamiltonian (Eqn. 1) with \( \gamma \) and \( \tau \) varies from 0 to \( \infty \). We performed UOD for Eqn. 5 using Genetic algorithm optimization [19]. In an operator optimization (as shown
in [19], optimization is performed for a constant unitary matrix—corresponds to a single fidelity point. Here optimization has to be performed for a two dimensional fidelity profile generated by $\gamma$ and $\tau$. We name it as Fidelity Profile Optimization (FPO). FPO for the present case is explained in following steps.

In the first step, we performed Fidelity Profile Optimization with following assumptions—(a). the range of $\tau$ is from 0 to 15, (b). the range of $\gamma$ is from 0 to 1 and (c). the system Hamiltonian ($H_{sys}$) is given by Eqn. 6

$$H_{sys} = H_{zz} = J_{zz}(\sigma_z \sigma_{zz}).$$

where $J_{zz}$ is the strength of $zz$-interaction.

The optimization procedure using Genetic algorithm is explained in the Supporting information.

The optimized UOD (Eqn. 7) has seven SQRs and two system Hamiltonian evolutions.

$$U(\gamma, \tau) = R^1(\frac{\pi}{2}, -\frac{\pi}{2}) R^1(\frac{\pi}{2}, \theta_2) R^2(\pi, \pi) U_{zz}(\frac{\pi}{2}) R^1(\theta_1, \theta_2 + \pi) R^2(\pi, \theta_2) U_{zz}(\frac{\pi}{2}),$$

where $\theta_1$ and $\theta_2$ (Eqn. 8) impart $\gamma$ and $\tau$ dependence to UOD and $U_{zz}$ is given by Eqn. 4 with $J_{zz} \times t = \pi/4$.

$$\theta_1 = [0.8423 - 0.3455 \cos(1.117\gamma) + 0.01806 \sin(1.117\gamma)] \tau,$$

$$\theta_2 = 1.345 \exp(-0.8731\gamma) + 1.796.$$  

The fidelity profile of UOD is shown in Fig. 1. The minimum point in fidelity profile is greater than 99.99 %. It should be noted that, the total length of UOD (Eqn. 7) is invariant under $\gamma$ and $\tau$ (with the assumption – all the SQRs are instantaneous).

For generalizing the assumption on $\tau$, we solved Eqn. 9 numerically and find the period $P(\gamma)$ of $U(\gamma, \tau)$ (Eqn. 10).

$$H(\gamma, \tau + n \times P(\gamma)) = H(\gamma, \tau).$$

$$P(\gamma) = 3.008 \gamma^3 - 6.627 \gamma^2 - 0.1498 \gamma + 12.59.$$  

Eqn. 10 has a maximum value of 12.59 at $\gamma=0$. Since the maximum value of period is less than 15 (FOP performed till $\tau=15$), UOD (Eqn. 7) can be used for any value of $\tau$. Same argument can be used for extending the range of $\tau$ to $-\infty$.

In order to incorporate the range of $\gamma$ from 0 to $\infty$, we performed FPO for the operator Eqn. 11.

$$U'(\gamma', \tau') = \exp(-i[\gamma'(\sigma_z \sigma_{2x} + \sigma_y \sigma_{2y}) + (\sigma_z \sigma_{2y} - \sigma_y \sigma_{2x}) \tau']),$$

and the optimized unitary decomposition are,

$$U'(\gamma', \tau') = R^1(\frac{\pi}{2}, \frac{\pi}{2}) R^2(\frac{\pi}{2}, \theta_3) R^1(\theta_2 + \theta_3, 0) R^1(\theta_1, \theta_4) U_{zz}(\frac{\pi}{2}) R^1(\frac{\pi}{2}, \frac{\pi}{2}) R^2(\frac{\pi}{2}, \theta_3),$$

where $\theta_1 \cdots \theta_4$ (Eqn. 12) impart $\gamma$ and $\tau$ dependence to UOD.

$$\theta = [0.09812 \exp(-2.42\gamma) + 0.4023 \exp(0.552\gamma)] \tau,$$

$$\theta_1 = -\theta + 3.142,$$

$$\theta_2 = \theta - [1.242 \exp(-0.961\gamma) + 0.3546 \exp(-0.1145\gamma)]$$

$$\theta_3 = 1.259 \exp(-0.957\gamma) + 3.479 \exp(-0.0087\gamma),$$

$$\theta_4 = 1.256 \exp(-0.959\gamma) + 1.912 \exp(-0.0166\gamma),$$

where $\gamma'$ varies from 0 to 1 and $\tau$ from 0 to 15.

Eqn. 11 satisfy the same periodicity relation as shown in Eqn. 10 and hence can use the same reasoning for extending $\tau$ range from 0 to $+\infty$.

For $\gamma > 1$, Eqn. 5 can be written as,

$$U'(\gamma'', \tau'') = \exp(-i[\gamma''(\sigma_z \sigma_{2x} + \sigma_y \sigma_{2y}) + (\sigma_z \sigma_{2y} - \sigma_y \sigma_{2x}) \tau'']),$$

where $\gamma'' = 1/\gamma$ and $\tau'' = \gamma \times \tau$.

Eqn. 11 and Eqn. 14 are equivalent and hence UOD for Eqn. 5 can be shown as,

$$U(\gamma, \tau) = \begin{cases} 
\text{Eqn. 5} & \text{if } \gamma \leq 1 \\
\text{Eqn. 11} & \text{if } \gamma > 1 
\end{cases}$$

The UOD optimization given Eqn. 7 is based on $H_{sys} = H_{zz}$ (Eqn. 6). It can be generalized to almost any interaction by term\ isolation procedure by Bremner et al. [20, 21].

As an example consider the case,

$$H_{sys} = J(\sigma_z \sigma_x + \sigma_y \sigma_y + \sigma_z \sigma_z).$$

The $H_{zz}$ terms can be isolated from Eqn. 10 and is shown in Eqn. 17.

$$\exp(-i J_{zz} \sigma_z \sigma_z t) = R^1(\pi, z) \exp(-i H_{sys} t) R^1(\pi, z),$$

where $R^1(\pi, z)$ represents a $\pi$-SQR on spin 1 along $Z$ axis.

Combining all the steps above forms most generic UOD of the Hamiltonian – DM interaction in the presence of Heisenberg XY interaction.
FIG. 2. $^{13}C$ labeled Chloroform used for quantum simulation. $^{13}C$ and $^1H$ act as qubits with zz interaction ($J_{CH}=215.1$ Hz) between them.

III. EXPERIMENTAL QUANTUM SIMULATION

We performed Quantum simulation experiments in a two qubit NMR system $^{13}CHCl_3$ (dissolved in Acetone-D6) (Fig. 2) with $^{13}C$ and $^1H$ spins act as two qubit system with scalar coupling (zz interaction– Eqn. 6) between them. The system Hamiltonian is zz interaction (Eqn. 6). We performed all the experiments in Bruker AV-500 spectrometer.

Quantum computation experiments in NMR starts with(i). preparation of pseudo pure states [22–24], (ii). processing the state by evolving under different average Hamiltonians [25] and (iii). read-out by quantum state tomography [26]. Here we studied the entanglement dynamics (quantified by concurrence [27]) of a Bell state (Eqn. 18) in the Hamiltonian given in Eqn. 1.

\[ |\phi\rangle_-=\frac{1}{\sqrt{2}}(|01\rangle-|10\rangle) \quad (18) \]

Using the unitary operator decompositions shown in Eqn. 15, we have simulated the Hamiltonian $H(\gamma, \tau)$ for $\gamma=\{0.33, 0.66, 0.99\}$ and studied the entanglement dynamics of the singlet Bell state (Eqn. 18) in the Hamiltonian given in Eqn. 1.

\[ AED = \sum_{i=1}^{n} \left| \frac{C_{es}(i) - C_{ts}(i)}{C_{ts}(i)} \right| \quad (19) \]

where $C_{es}(i)$ and $C_{ts}(i)$ are the concurrence in experimental and theoretical simulations and $n$ is the number of experimental points (here we performed simulation for $n=16$).

FIG. 3. (a). Entanglement (concurrence) dynamics of $^{13}C-H$ system under the Hamiltonian Eqn. 1. (b). Entanglement preservation experiment using Eqn. 20. Starting from singlet state, the concurrence sustains at 1 with the preservation procedure.

1. **Entanglement Preservation**

Hou et al. [29] demonstrated a mechanism for entanglement preservation of a quantum state in a Hamiltonian of the type given in Eqn. 2.

Preservation of initial entanglement of a quantum state is performed by free evolution interrupted with a certain operator $O$, which makes the state to go back to its initial state. The operator sequence for preservation is given in Eqn. 20

\[ OU(\gamma, \tau)OU(\gamma, \tau) \equiv I, \quad (20) \]

where $O = I_1 \otimes \sigma_{2z}$.

We performed entanglement preservation experiment for singlet state (Eqn. 18) in $H(\gamma, \tau)$ with $\gamma=\{0.33, 0.66, 0.99\}$. The experimental results (Fig. 3(b)) shows excellent entanglement preservation and good agreement with the theoretical simulation. The experimental deviation of concurrence (Eqn. 19) is less than 2%.
CONCLUSION

We have performed Fidelity Profile Optimization for the Hamiltonian – DM interaction in the presence of Heisenberg XY interaction. The optimized UOD can be used for all relative strengths ($\gamma$) of the interactions and length is invariant under $\gamma$ or evolution time. Using these decompositions, we have experimentally verified the entanglement preservation mechanism suggested by Hon et al.

ACKNOWLEDGMENTS

We thank Prof. Apoorva Patel for discussions and suggestions, and the NMR Research Centre for use of the AV-500 NMR spectrometer. V.S.M. thanks UGC-India for support through a fellowship.

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