Simulating decoherence behavior of a system in entangled state using nuclear magnetic resonance

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Abstract
By choosing $^1H$ nucleus in Carbon-13 labelled trichloroethylene as one qubit environment, and two $^{13}C$ nuclei as a two-qubit system, we have simulated quantum decoherence when the system lies in an entangled state using nuclear magnetic resonance (NMR). Decoupling technique is used to trace over the environment degrees of freedom. Experimental results show agreements with the theoretical predictions. Our experiment scheme can be generalized to the case that environment is composed of multiple qubits.

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Quantum decoherence is a purely quantum-mechanical effect through which a system loses its coherence behavior by getting entangled with its environment degrees of freedom [1][2]. A real quantum system always interacts with its surrounding environment. The time evolution induced by the interaction introduces entanglement between the system and environment when the system initially lies in a superposition of states. When the state of the system is described by a reduced density matrix through tracing over the environment degrees of freedom, decoherence makes the off-diagonal matrix elements approach 0, and leaves diagonal ones unaltered. Quantum decoherence is thought as a main obstacle for experimental imple-
mentations of quantum computation and has been widely studied in theory [3]-[5]. Some theoretical and experimental schemes have also been proposed to solve the problem of decoherence in order to fully use coherence in quantum information[6]-[8]. C.J. Myatt. et al observed and studied decoherence by coupling an ion in a Paul trap to a reservoir that can be controlled[9][10]. D. G. Cory et al simulated decoherence by magnetic field gradients [7]. In this paper, we will simulate decoherence when the system lies in an entangled state. Although we choose one qubit to simulate the environment, our scheme can be generalized to the case that the environment is composed of multiple qubits.

We choose carbon 13-labelled trichloroethylene (TCE) dissolved in d-chloroform as a sample. TCE’s structure is shown in Fig.1. The two $^{13}$C nuclei constitute the system, and the $^1$H nucleus is viewed as environment. They represent qubits 1, 2, and 3, respectively. The influence of the other nuclei can be ignored. The Hamitonian of the system and environment is represented as

$$H_{s+e} = -\omega_1 I_1^z - \omega_2 I_2^z - \omega_3 I_3^z + 2\pi J_{12} I_1^z I_2^z + 2\pi J_{23} I_2^z I_3^z + 2\pi J_{13} I_1^z I_3^z,$$  \hspace{1cm} (1)

where $\omega_k/2\pi (k = 1, 2, 3)$ are the resonance frequencies of the 3 spins, $I_z^k$ are the matrices for the z-components of the angular momentum, and $\hbar$ is set
to 1, \(J_{12}\), for example, denotes the coupling constant between spins 1 and 2. Before the system lies in an entangled state, \(^1\)\(H\) nucleus is decoupled. \(J_{23}\) and \(J_{13}\) are averaged to zero. The system becomes a closed system whose Hamiltonian is represented as

\[
H_s = -\omega_1 I_z^1 - \omega_2 I_z^2 + 2\pi J_{12} I_z^1 I_z^2. \tag{2}
\]

According to Ref.[11] and the experimental technique we used for heteronuclear system [12], the pulse sequence \([\alpha]_{z}^2 - [\text{grad}]_z - [\pi/4]_{x}^2 - 1/4J_{12} - [\pi]_{y}^2 - 1/4J_{12} - [-5\pi/6]_{y}^1 - [\text{grad}]_z\) transforms the system from equilibrium state to the pseudo-pure state \(\downarrow^1 \downarrow^2\) represented as \(\rho_{ef} = I_z^1 + I_z^2 - 2I_z^1 I_z^2\).

Here \([\alpha]_{z}^2\), for example, refers to a radio-frequency (rf) pulse on spin 2, oriented along x-axis. The evolution caused by the pulse is denoted as \(e^{i\alpha I_z^2}\). \([\text{grad}]_z\) denotes a gradient pulse along z-axis. \(1/4J_{12}\) denotes the evolution caused by \(H_s\) for \(1/4J_{12}\) without pulses. Because of the difference of abundance of \(^{13}\)\(C\)1 and \(^{13}\)\(C\)2 in the sample and the effects caused by decoupling, the equilibrium state of the system is represented as \(\gamma_C^1 I_z^1 + \gamma_C^2 I_z^2\), instead of \(\gamma_C(I_z^1 + I_z^2)\), where \(\gamma_C\) is the gyromagnetic ratio of \(^{13}\)\(C\) nucleus. We call \(\gamma_C^1\) and \(\gamma_C^2\) ”effective gyromagnetic ratios” for \(^{13}\)\(C\)1 and \(^{13}\)\(C\)2, respectively.

\(\alpha = \arccos(\gamma_C^1/\gamma_C^2)\), where \(\gamma_C^1/\gamma_C^2\) can be measured by experiment.

The pulse sequence \([\pi/2]_{x}^1 - [\pi/4]_{x}^2 - [\pi]_{x}^1 - [\pi/2]_{y}^2\) transforms \(\downarrow^1 \downarrow^2\)
into an entangled basis state [13]

\[
\rho_s(0) = I_x^1 I_x^2 - I_z^1 I_z^2 - I_y^1 I_y^2, \tag{3}
\]

As soon as the system lies in the entangled state, the decoupling pulses are closed. The system and environment evolve under \( H_{s+e} \). By applying a hard (nonselective) pulse \([\pi]_{1,2,3}^x\) in the middle of a period of evolution time \( t \) (shown in Fig.2), the effect of chemical shift evolution during this period can be cancelled [14][15]. The system evolves under \( H_{ef} \) represented as

\[
H_{ef} = 2\pi J_{12} I_x^1 I_x^2 + 2\pi J_{23} I_z^2 I_z^3 + 2\pi J_{13} I_z^1 I_z^3, \tag{4}
\]

where the last two terms describe the interaction between the system and environment. Only these two terms cause the system to evolve, because entangled basis states are the eigenstates of \( I_z^1 I_z^2 \) [16]. After \( t \), the environment degrees of freedom are introduced into the density matrix of the system described as

\[
\rho_s(t, I_z^3) = \cos(\varphi_{13} + \varphi_{23})(I_x^1 I_x^2 - I_y^1 I_y^2) - I_z^1 I_z^2 + 2\sin(\varphi_{13} + \varphi_{23})(I_x^1 I_y^2 + I_y^1 I_x^2) I_z^3, \tag{5}
\]

where \( \varphi_{13} = \pi J_{13} t \), and \( \varphi_{23} = \pi J_{23} t \). By tracing over the environment degrees of freedom, the density matrix of the system is obtained, which is represented
as

\[
\rho_s(t) = 3\left| \rho_s(t, I_z^3) \right| \uparrow >_3 + 3 \left| \rho_s(t, I_z^3) \right| \downarrow >_3 = \cos(\varphi_{13} + \varphi_{23})(I_x^1 I_x^2 - I_y^1 I_y^2 - I_z^1 I_z^2),
\]

(6)

using \( I_z^3 \left| \uparrow >_3 = \frac{1}{2} \left| \uparrow >_3 \right. \), and \( I_z^3 \left| \downarrow >_3 = -\frac{1}{2} \left| \downarrow >_3 \right. \). In NMR experiments, Eq.(6) is equivalent to the deviation density matrix [13] represented as

\[
\rho_s(t) = \begin{pmatrix}
1 & 0 & 0 & -\cos(\varphi_{13} + \varphi_{23}) \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
-\cos(\varphi_{13} + \varphi_{23}) & 0 & 0 & 1
\end{pmatrix},
\]

(7)

where basis states are arrayed as \( | \uparrow >_1 | \uparrow >_2, | \uparrow >_1 | \downarrow >_2, | \downarrow >_1 | \uparrow >_2, \)

\( | \downarrow >_1 | \downarrow >_2 \). For convenience, we also use \( \rho_s(t) \) in Eq.(7). The function \( \cos(\varphi_{13} + \varphi_{23}) \) describes the decoherence behavior which can be observed in the NMR spectrum through a readout pulse \( [\frac{\pi}{2}]_x \) which transforms the system into the state represented as

\[
\rho_{sr}(t) = \begin{pmatrix}
0 & i & -\cos(\varphi_{13} + \varphi_{23}) & \cos(\varphi_{13} + \varphi_{23}) \\
-i & 0 & \cos(\varphi_{13} + \varphi_{23}) & i \cos(\varphi_{13} + \varphi_{23}) \\
i \cos(\varphi_{13} + \varphi_{23}) & \cos(\varphi_{13} + \varphi_{23}) & 0 & -i \\
\cos(\varphi_{13} + \varphi_{23}) & -i \cos(\varphi_{13} + \varphi_{23}) & i & 0
\end{pmatrix}.
\]

(8)
Experimental data are taken at controlled temperature (22\textdegree\text{C}) with a Bruker DRX 500 MHz spectrometer. The coupling constants $J_{12} = 103.1\text{Hz}$, $J_{23} = 201.3\text{Hz}$, and $J_{13} = 9.23\text{Hz}$. $^1\text{H}$ nucleus is again decoupled during recording the FID signal. In our experiments, decoupling is the process of tracing over the environment degrees of freedom to get the reduced density matrix of the system, i.e., Eq.(6) is obtained from Eq.(5). Fig.3a is the carbon spectrum through the readout pulse $\left[\frac{\pi}{2}\right]_x$ when $t = 3.50\text{ms}$. The center frequencies of $^{13}\text{C}1$ and $^{13}\text{C}2$ are 124.16 ppm and 117.00 ppm, respectively. Fig.3b shows that the amplitude of the left peak of $^{13}\text{C}1$ varies as $t$. The experimental data points can be fitted as function $5.8\cos(2\pi t/T)$, where $T = 8.72\text{ms}$. In theory, $T = 9.50\text{ms}$. The error is about 8.2\%. It mainly results from the imperfection of pulses, and the effect of decoherence which cannot be controlled.

If environment is composed of multiple qubits, the interaction between the system and environment is represented as

$$ H_i = \sum_{k=3}^{N+2} (2\pi J_{1k} I^1_z I^k_z + 2\pi J_{2k} I^2_z I^k_z). $$

(9)

Under the evolution induced by $H_i$, the system is described as

$$ \rho_s(t) = I^1_x I^2_x \prod_{k=3}^{N+2} \cos(\varphi_{1k} + \varphi_{2k}) - I^1_z I^2_z - I^1_y I^2_y \prod_{k=3}^{N+2} \cos(\varphi_{1k} + \varphi_{2k}), $$

(10)
through tracing over environment degrees of freedom, where $\varphi_{1k} = \pi J_{1k} t$, and $\varphi_{2k} = \pi J_{2k} t$. If $N \to \infty$, the coherence usually approaches to 0 very fast, if $t \neq 0$.

In our experiments, we examine quantum decoherence of a system in an entangled state. It is unnecessary to consider the state of environment. In fact, we usually cannot describe the state of environment clearly. The interaction between the system and environment introduces the environment degrees of freedom into the state of the system. Decoherence is the result of tracing over such degrees of freedom.

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Figure Captions

1. The structure of trichloroethylene. The two $^{13}C$ nuclei and one $^1H$ nucleus represent qubits 1, 2, and 3, respectively.

2. The scheme used to cancel the chemical shift evolution. $t$ denotes the evolution time. Nonselective $\pi$ pulses are applied in the middle of $t$.

3. The experimental results when the two $^{13}C$ nuclei in an entangled state evolute under $H_{ef}$ (see the text). $^1H$ nucleus is decoupled during recording the FID signal. Fig.3a is the carbon spectrum through a readout pulse $[\frac{\pi}{2}]_2$ when $t = 3.50$ ms. The center frequencies of $^{13}C1$ and $^{13}C2$ are 124.16 ppm and 117.00 ppm, respectively. Fig.3b shows that the amplitude of the left peak of $^{13}C1$ varies as $t$. The experimental data points can be fitted as function $5.8cos(2\pi t/T)$, where $T = 8.72ms$.

[Figure 1 about here.]

[Figure 2 about here.]

[Figure 3 about here.]
List of Figures

1 ..................................................... 13
2 ..................................................... 14
3 ..................................................... 15
Figure 1:
Figure 2:
Figure 3: