Journal of Magnetic Resonance 198 (2009) 248–251

Contents lists available at ScienceDirect

Journal of Magnetic Resonance

journal homepage: www.elsevier.com/locate/jmr

Projection of a quantum state on eigenstates of average Hamiltonian

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ARTICLE INFO

Article history:
Received 1 November 2008
Revised 14 February 2009
Available online 5 March 2009

Keywords:
Average Hamiltonian
Bell states
Projection
Dipolar-coupled
Liquid crystal

ABSTRACT

A scheme for projecting an arbitrary quantum state on eigenstates of average Hamiltonian is described. As an experimental example, projection on entangled Bell states, which are eigenstates of specially constructed average Hamiltonian, is demonstrated for a system of two dipolar-coupled nuclear spins. The results of a direct and time-reversed evolution are added to average out the coherences between different eigenstates and accomplish the projection.

Nuclear magnetic resonance (NMR) has been an outstanding testbed for implementing controlled dynamics [1–4] in systems of up to twelve coupled nuclear spins [5–7]. A flexibility of NMR in handling spin dynamics comes from possible fast modulation of internal interactions by external radio-frequency fields. Such modulation allows "switching" interactions on and off or, more generally, creating average [8] or effective [9] Hamiltonians, which naturally do not exist [10,11]. Average Hamiltonians with specially designed spectral properties are commonly used in NMR spectroscopy. One can also think about constructing average Hamiltonians with desired eigenstates, including the states which are not eigenstates of any naturally existing Hamiltonians. As we will show, projection on the eigenstates of such Hamiltonian can be an efficient method of extracting information about quantum states.

In quantum mechanics, any observable physical quantity can be represented by a Hermitian operator [12]. However, there is no general approach for designing a measurement that projects a state onto eigenstates of an arbitrary Hermitian operator. When it is necessary to perform a projection on the states that are not eigenstates of some observable, the results of such projection are reconstructed indirectly by applying a set of unitary transformations to a projected state [13–15]. This procedure constitutes a basis for the state reconstruction. More direct way to project a given quantum state onto arbitrary states would be creating an average Hamiltonian with desired eigenstates and averaging out the coherences between different eigenstates of this average Hamiltonian. The experimental illustration below is based on creating an average Hamiltonian with non-degenerate eigenvalues and Bell eigenstates.

Four entangled Bell states of a two-qubit system, or a system of two spins ½, are $|\Phi_{\pm}\rangle = 2^{-1/2}\ (|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle)$ and $|\Psi_{\pm}\rangle = 2^{-1/2}\ (|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)$, where $|\uparrow\rangle$ ($|\downarrow\rangle$) indicate the state with a spin up (down). They have played an important role in exploring differences between quantum and classical physics, formulating the Bell inequalities [16], or the EPR paradox [17], discussions on non-locality and hidden variables [18,19]. Discrimination between the Bell states is an important measurement in quantum communication. As an example, the protocols of dense coding [20], quantum teleportation [21], and entanglement swapping [22] require a projective measurement in the Bell basis. Until now, such measurement remained a *gedanken* experiment, and there have been no physical realizations of the direct projective measurement in the Bell basis. Experimental discrimination between the Bell states has been achieved by joint measurements with probabilistic success [23] or by disentangling the Bell states into separable states [24–28].

In this paper, we describe a direct projection onto the Bell states for a system of two dipolar-coupled nuclear spins. Due to the ensemble nature of NMR experiments, we can describe the projection in terms of a density matrix. Measurement in NMR is a weak ensemble measurement. However, the experiment can be designed to extract the results of projective quantum measurement: possible outcomes and corresponding probabilities [29].

The average Hamiltonian with Bell eigenfunctions H_{Bell} can be constructed as follows. Suppose that the eigenvalues corresponding to the eigenvectors $2^{-1/2}\ (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$, $2^{-1/2}\ (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)$, $2^{-1/2}\ (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, and $2^{-1/2}\ (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ are, respectively, *a*, *b*, *c*, and *d*. In the multiplicative basis, the Bell Hamiltonian H_{Bell} can be obtained by a unitary transformation

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doi:10.1016/j.jmr.2009.02.013

$$H_{\mathrm{Bell}} = \frac{1}{\sqrt{2}}\begin{pmatrix}1&1&0&0\\0&0&1&1\\0&0&1&-1\\1&-1&0&0\end{pmatrix}\begin{pmatrix}a&0&0&0\\0&b&0&0\\0&0&c&0\\0&0&0&d\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1&0&0&1\\1&0&0&-1\\0&1&1&0\\0&1&-1&0\end{pmatrix} = \frac{1}{2}\begin{pmatrix}a+b&0&0&a-b\\0&c+d&c-d&0\\0&c-d&c+d&0\\a-b&0&0&a+b\end{pmatrix}, \quad (1)$$

or, by using the Pauli spin operators,

$$H_{\mathrm{Bell}} = 4^{-1}[(a+b+c+d)\mathbf{1} + (a+b-c-d)\sigma_{1z}\sigma_{2z} + (a-b+c-d)\sigma_{1x}\sigma_{2x} + (-a+b+c-d)\sigma_{1y}\sigma_{2y}], \quad (2)$$

where $\mathbf{1}$ is the identity operator. The terms of this Hamiltonian can be built from the dipole–dipole and the double-quantum Hamiltonians. At $a = -b$ and $d = 0$

$$H_{\mathrm{Bell}} = 2^{-1}c\mathbf{1} - 4^{-1}c(\sigma_{1z}\sigma_{2z} - \sigma_{1x}\sigma_{2x} - \sigma_{1y}\sigma_{2y}) + 2^{-1}a(\sigma_{1x}\sigma_{2x} - \sigma_{1y}\sigma_{2y}) = 2^{-1}c\mathbf{1} - 2^{-1}cH_{zz} + (a/3)(H_{xx} - H_{yy}), \quad (3)$$

where $H_{zz} = \sigma_{1z}\,\sigma_{2z} - 2^{-1}$ ($\sigma_{1x}\,\sigma_{2x} + \sigma_{1y}\,\sigma_{2y}$) is the secular Hamiltonian of dipole–dipole interaction between spins 1 and 2, $H_{xx} = \sigma_{1x}\,\sigma_{2x} - 2^{-1}$ ($\sigma_{1y}\,\sigma_{2y} + \sigma_{1z}\,\sigma_{2z}$), $H_{yy} = \sigma_{1y}\,\sigma_{2y} - 2^{-1}$ ($\sigma_{1z}\,\sigma_{2z} + \sigma_{1x}\,\sigma_{2x}$), and $H_{xx} - H_{yy}$ is a pure double-quantum Hamiltonian. The Hamiltonian proportional to $H_{xx} - H_{yy}$ can be obtained from H_{zz} by applying the multi-pulse sequence with eight-pulse cycle [30]. The Bell Hamiltonian H_{Bell} in Eq. (3) has an additional H_{zz} term and, therefore, can be obtained by changing relative intervals between pulses in the eight-pulse sequence. Parameters of the pulse sequence can be optimized by a computer simulation which takes into account difference of chemical shifts for the spins and finite duration of the pulses.

Below we present the results for the case when the initial state is in the subspace spanned by only two of the Bell states $|\Phi_{\pm}\rangle = 2^{-1/2}(|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle)$. This case is especially simple for experimental realization but well illustrates the principle. The physical system contained 2% of 1-dodecene-1,2-$^{13}C_2$ dissolved in liquid crystal 4′-pentyl-4-cyanobiphenyl (5CB). Under proton decoupling, ^{13}C nuclei of the same molecule form isolated spin pairs with residual dipolar coupling between the spins of the same pair. The experiment has been performed with a Varian Unity/Inova 500 MHz NMR spectrometer at 23 °C. At this temperature, the chemical shift difference between two ^{13}C spins is 3 kHz. The splitting due to the coupling is 353 Hz, and ^{13}C NMR lines from the 1-dodecene-1,2-$^{13}C_2$ molecules and 5CB do not overlap.

The pulse sequence is shown in Fig. 1(a). The first step, not shown in the figure, is the ^{13}C polarization enhancement by cross-polarization from protons, performed by two simultaneous frequency-sweeping pulses [31]. The resulting spectrum is shown in Fig. 1(b). During the step A, the pseudopure ground state $|\uparrow\uparrow\rangle$ is created by using a partial saturation. A two-frequency irradiation of 5 ms duration at the resonance frequencies of transitions between states $|\uparrow\downarrow\rangle$ and $|\downarrow\downarrow\rangle$ and between states $|\downarrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ (indicated by two arrows in Fig. 1(b)) equalizes the populations of three states other than the ground state $|\uparrow\uparrow\rangle$. Unwanted coherences between states are removed by a z-filter, implemented by turning off the ^1H decoupling [32] for 1 ms after the two-frequency pulse. This elimination of coherences is very efficient, as evidenced by the linear-response spectrum in Fig. 1(c) and the reconstructed density matrix of the pseudopure ground state in Fig. 2(a). For the state reconstruction we used the protocol described in Ref. [33]. When needed, the Bell states $|\Phi_{\pm}\rangle$ can be obtained from the ground state by using a sequence of rf pulses and delays, as it is shown in step B of Fig. 1(a). The sequence is $(\pi/2)_{\mathrm{h}} - (\tau/2) - (\pi)_{\mathrm{h}} - (\tau/2) - (\pi/2)_{\mathrm{s}}$, where $(\pi/2)_{\mathrm{h}}$ and $(\pi)_{\mathrm{h}}$ are, respectively, non-selective 90° and 180° pulses, $(\pi/2)_{\mathrm{s}}$ is a selective pulse on either of two ^{13}C spins, and $\tau = 1/(2 \times 353\ \mathrm{Hz})$ is the delay producing the phase gate: $|\uparrow\uparrow\rangle \to |\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle \to |\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle \to |\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle \to -|\downarrow\downarrow\rangle$. The reconstructed density matrix for one of the Bell states $|\Phi_{+}\rangle = 2^{-1/2}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$ is shown in Fig. 3(a).

The state projection is performed in step C of Fig. 1(a). For the subspace of states $|\Phi_{\pm}\rangle$ one can use the original eight-pulse sequence [30] without any modification. This sequence creates the double-quantum average Hamiltonian with Bell eigenstates. However, two of them $|\Psi_{\pm}\rangle = 2^{-1/2}(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)$ are degenerate and cannot be distinguished. The states $|\Phi_{\pm}\rangle$ have different eigenvalues λ_1 and λ_2. Due to finite pulse durations, one of the eigenstates is slightly different from the state $|\Phi_{+}\rangle$ (theoretical fidelity was 0.91) while the other eigenstate is always identical to the state $|\Phi_{-}\rangle$. The total duration of two cycles of the eight-pulse sequence $t = 1.5$ ms has been adjusted to give $t(\lambda_1 - \lambda_2) = \pi/2$. The eigenvalues λ_1 and λ_2 have been calculated numerically by estimating the evolution operator of the original eight-pulse sequence. In this calculation, we used experimental values of chemical shifts, coupling constant, and pulse durations. Change of sign of the double-quantum average Hamiltonian, or reversed evolution, can be achieved by shifting the phases of all pulses in the eight-pulse sequence by $\pi/2$. Elimination of the coherences was done by adding the results from the forward and time-reversed evolutions after the evolution time $t = (\pi/2)(\lambda_1 - \lambda_2)^{-1}$, which produced the relative phase π between the coherences. As a result, the coherences between two Bell states $|\Phi_{\pm}\rangle$ have been canceled out and the projection accomplished. In a more general case involving all four Bell states, elimination of coherences can be done with an array of evolution times, similar to used in Ref. [5] for averaging out the unwanted coherences.

In step D (Fig. 1(a)), a set of the NMR signals was acquired to reconstruct the density matrix. The result of projective quantum measurement can be extracted from NMR experiment in a simpler way [29]. Here we present all elements of the density matrix to verify the accuracy of the projection. Figs. 2 and 3 show the results for the initial ground state $|\uparrow\uparrow\rangle$ (without step B) and the Bell state $|\Phi_{+}\rangle$ (with step B) before and after the projection. The reconstructed density matrices are presented in both multiplicative and Bell bases. As one can see in Fig. 2(a), the density matrix of the ground state $|\uparrow\uparrow\rangle$ has only one diagonal element in the multiplicative basis. At the same time, this state is a superposition of two Bell states (Fig. 2(a′)). The result of projecting this state onto the Bell basis is shown in Fig. 2(b) and (b′). Since the ground state is a superposition of two Bell states: $|\uparrow\uparrow\rangle = 2^{-1/2}(|\Phi_{+}\rangle + |\Phi_{-}\rangle)$, it is expected that, after the projection, the system would end in the mixed state $2^{-1}(|\Phi_{+}\rangle\langle\Phi_{+}| + |\Phi_{-}\rangle\langle\Phi_{-}|)$. The experiment confirms that the system is in the desired mixed state presented in Fig. 2(b′): the density matrix in the Bell basis has two diagonal and no off-diagonal elements. Simultaneously, this state is a mixture of the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$, as one can see in Fig. 2(b).

If the state before projection is one of the Bell states, one would expect that projection on the Bell states would leave the state unchanged. The results of this test are shown in Fig. 3. The experiment is exactly the same as described above, except that the initial state is the Bell state $|\Phi_{+}\rangle$. The density matrix has only one diagonal element in the Bell basis (Fig. 3(a′)) and has a superposition form in the multiplicative basis (Fig. 3(a)). The result of projection shown in Fig. 3(b) and (b′) confirms that the state is preserved.

In conclusion, average Hamiltonians, resulting from averaging fast-modulated internal interactions, can be designed to have desired eigenstates. A state of a system can be projected on these eigenstates of the average Hamiltonian. As an example, we have demonstrated projection of a state of a two-spin system onto the

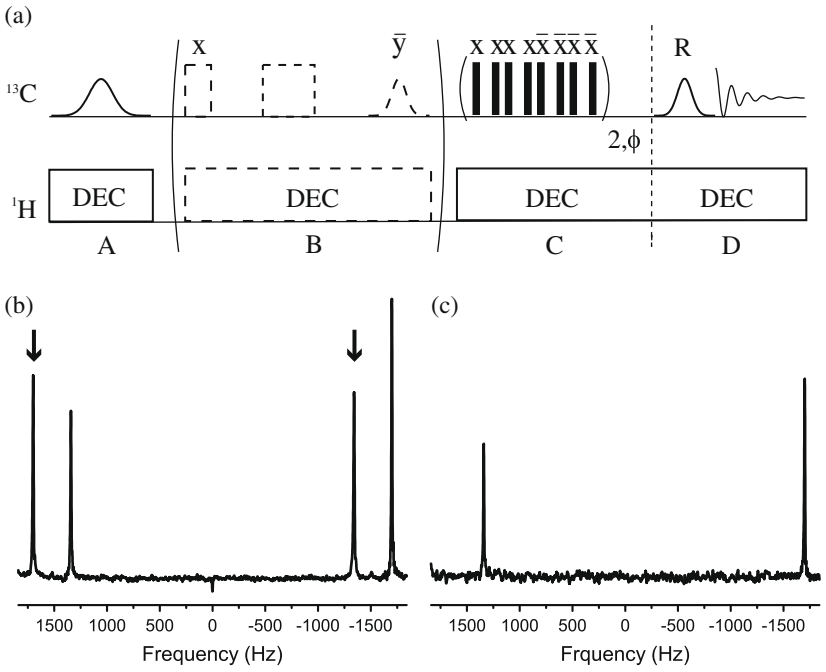

Fig. 1. (a) NMR pulse sequence. (b) ^{13}C NMR spectrum obtained with a 90° hard pulse. The polarization of ^{13}C spins has been enhanced by cross-polarization. (c) ^{13}C NMR linear-response spectrum of the pseudopure state $|\uparrow\uparrow\rangle$. The vertical scale for this spectrum is increased by a factor 4.

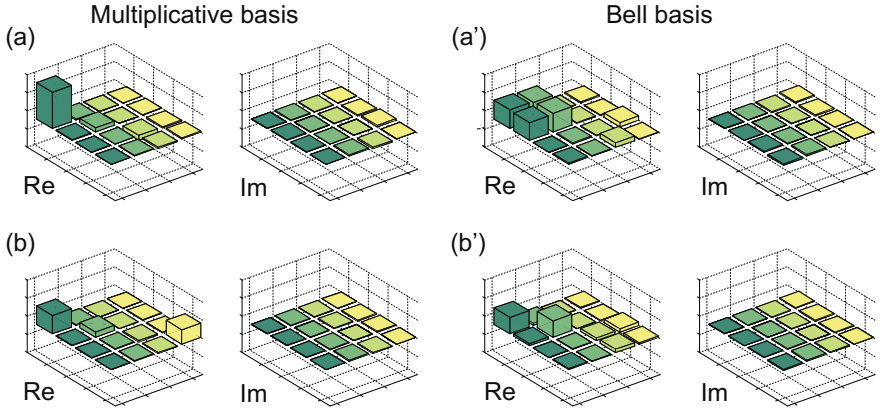

Fig. 2. Reconstructed density matrices for the initial ground state $|\uparrow\uparrow\rangle$ before (a) and after (b) projection on Bell states.

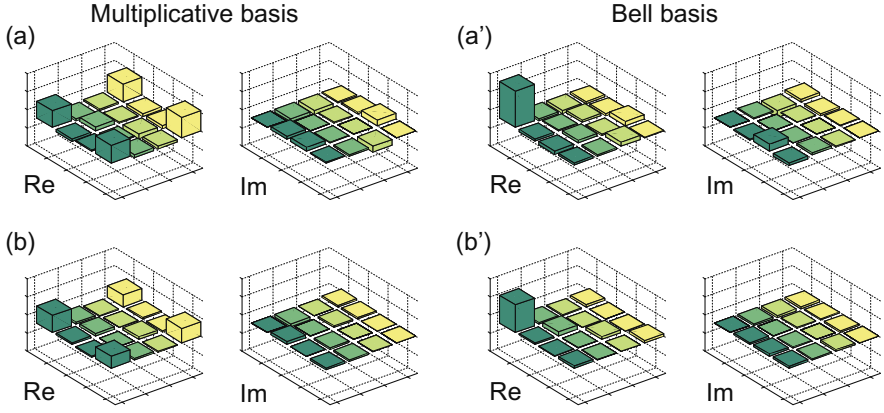

Fig. 3. Reconstructed density matrices for the initial Bell state $|\Phi_+\rangle$ before (a) and after (b) projection on Bell states.

Bell states, which are not eigenstates of any naturally existing Hamiltonian.

Acknowledgment

This work was supported in part by the NSF under Grant No. ECS-0608846.

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