Simulations of Information Transport in Spin Chains

P. Cappellaro,[1] C. Ramanathan,[2] and D. G. Cory[2]

[1]ITAMP-Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA

[2]Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

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Transport of quantum information in linear spin chains has been the subject of much theoretical work. Experimental studies by NMR in solid state spin systems (a natural implementation of such models) is complicated since the dipolar Hamiltonian is not solely comprised of nearest-neighbor XY-Heisenberg couplings. We present here a similarity transformation between the XY Hamiltonian and the double-quantum Hamiltonian, an interaction which is achievable with the collective control provided by radio-frequency pulses. Not only can this second Hamiltonian simulate the information transport in a spin chain, but it also creates coherent states, whose intensities give an experimental signature of the transport. This scheme makes it possible to study experimentally the transport of polarization beyond exactly solvable models and explore the appearance of quantum coherence and interference effects.

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In many solid state proposals for quantum information processing an essential task is the transport of information over relatively short distances. Today there are no proven schemes for accomplishing this chore despite many promising proposals. One approach is to use linear spin chains coupled by the XY-Heisenberg Hamiltonian [1,2]. Various protocols have been proposed to obtain perfect state transfer in this system, involving engineering the couplings [3] or the Hamiltonian [4]. Usually these schemes are based on nearest-neighbor (NN) couplings, which allow for analytical solutions of the dynamics. Beyond the 1D, NN limit, the dynamics becomes richer and quantum interferences appear. Experimental studies would enable us to go beyond this limit, while keeping the fundamental symmetries of the Hamiltonian. While optical lattices have been proposed as versatile quantum simulators for a variety of spin Hamiltonians [5], here we propose to use a system closer to the simulated one—a pseudo-1D dipole coupled spin chain—taking advantage of the control methods developed by the NMR community to explore dynamics close to the solvable model. In addition, a quantum simulation of this transport mechanism will connect to studies of spin diffusion [6].

In this Letter we show how well-known NMR pulse sequences can be used to experimentally study the transport of quantum information, in collectively controlled, room temperature linear spin chains. Quasi-1D spin systems are available in some materials like apatites [7]. We first introduce a Hamiltonian [the so-called double-quantum (DQ) Hamiltonian] that is connected to the XY-Hamiltonian by a similarity transformation and is obtained experimentally by sequences of pulses and delays in dipolar spin systems. We show how this Hamiltonian can simulate the transport dynamics for relevant initial states, by comparing the probability of transfer for the two Hamiltonians. We show furthermore that the DQ Hamiltonian enables the detection of successful transport, even if it is not possible to measure single nuclear spins. Although the experiment we propose is an approximation of the ideal model (and as such is not an implementation of a quantum information bus) it permits the experimental study of perturbations to this model, such as contributions from next-nearest neighbors or other chains, that yield a richer physics (for example, a crossover to nonintegrable systems [8]).

Transport of Zeeman and dipolar energy in spin systems, caused by energy conserving spin flips, has been a long term interest in spin physics and more recently in quantum information science [9,10]. The evolution of the system induced by the secular dipolar Hamiltonian $\mathcal{H}_{\text{dip}} = \sum_{ij} d_{ij}[\sigma_z^i\sigma_z^j - \frac{1}{2}(\sigma_x^i\sigma_x^j + \sigma_y^i\sigma_y^j)]$, is coherent (as proved by the observation of polarization echoes [11]), but the complexity of the interaction encodes information about the created many-body states in observables that are not directly measurable in NMR experiments. The free-evolution transport presents the signature of an apparent diffusive behavior [6], with an effective decay time T_2^* much shorter than spin-lattice relaxation times. Refocusing experiments can extend the transverse relaxation T_2 to much larger values, although still quite far from the theoretical limit of the longitudinal relaxation T_1. If no special assumptions are made on the values of the dipolar couplings [12] or the initial state [13], spin diffusion (that is, evolution under the secular dipolar Hamiltonian) cannot transfer the polarization from the first to the last spin with any appreciable efficiency [14], even for a small number of spins in linear chains. On the other hand, a simpler Hamiltonian, the NN XY interaction,

$$\mathcal{H}_{\text{xy}} = \sum_i \frac{d}{2}(\sigma_x^i\sigma_x^{i+1} + \sigma_y^i\sigma_y^{i+1}) = \sum_i d(\sigma_+^i\sigma_-^{i+1} + \sigma_-^i\sigma_+^{i+1}),$$

has been studied extensively for perfect transport purposes, but it is not found naturally in spin systems. It has been shown that perfect transport of a state is possible only for chains up to 3 spins [3], but if one can engineer the coupling strength [15] or add external manipulation of all the spins [16] or even just of the spins at the chain ends [17], perfect transport is achievable for chains of arbitrary length.

Unfortunately, given the dipolar Hamiltonian it is impossible with only collective control to obtain the XY-Hamiltonian. With collective control, by means of a sequence of radio-frequency (rf) pulses and delays [18], we can create the DQ Hamiltonian:

$$\mathcal{H}_{\mathsf{dq}} = \sum_{ij} \frac{d_{ij}}{2}(\sigma_x^i\sigma_x^j - \sigma_y^i\sigma_y^j) = \sum_{i,j} d_{i,j}(\sigma_+^i\sigma_+^j + \sigma_-^i\sigma_-^j).$$

A simple unitary transformation links the DQ and XY Hamiltonians if we restrict the couplings to the nearest-neighbor spins [19]. The transformation, however, cannot be obtained by an rf pulse sequence, since it is not a collective operation:

$$\mathcal{H}_{\mathsf{xy}} = U_{\mathsf{dq}}^{\mathsf{xy}}\mathcal{H}_{\mathsf{dq}}(U_{\mathsf{dq}}^{\mathsf{xy}})^\dagger, \qquad U_{\mathsf{dq}}^{\mathsf{xy}} = \exp\left(-i\frac{\pi}{2}\sum_k{}' \sigma_x^k\right),$$

where the sum is restricted to either even or odd spins.

Since the two Hamiltonians are related by a similarity transformation, the DQ Hamiltonian (experimentally available) can simulate the dynamics of the XY Hamiltonian, provided one can prepare initial states and detect observables which are invariant under the transformation. With these assumptions, even if the similarity transformation $U_{\mathsf{dq}}^{\mathsf{xy}}$ is not explicitly applied, the evolution of these particular initial states is the same. For thermally polarized spin systems at $T > 100$ mK, an obtainable initial state relevant to this problem is to have just one-spin polarized [20], $\rho(0) = (\mathbb{1}_a + \frac{\hbar\omega}{k_b T}\sigma_a^z) \otimes \mathbb{1}_{N\neq a}$ (in the following we will only consider the deviation of the density matrix from identity, which is its only experimentally observable part). Since this state is invariant under the transformation $U_{\mathsf{dq}}^{\mathsf{xy}}$, the DQ-Hamiltonian opens the possibility to experimentally study spin transport in dipolarly coupled systems. Incidentally, the pure state usually considered in theoretical studies—the one-spin excitation state—is not invariant under the transformation.

Notice that the relationship between the XY and DQ Hamiltonian is also valid in two and three dimensions (and in general on hypercubes of any dimensions, which have already been shown to allow perfect state transport under the XY interaction [15]). These spin systems can be thought of as treelike graphs [21]. A spin at one edge of the D-dimension hypercube is at the top of the tree, and has D neighbors in the following level; in general each node has D links to the upper and lower levels. The similarity transformation is performed by flipping all the spins of either the odd or even levels.

We study the polarization transfer given by the XY and DQ Hamiltonian, when the transformation $U_{\mathsf{dq}}^{\mathsf{xy}}$ is not explicitly applied (as in experiments). The dynamics is solved in terms of fermion operators and of their Fourier transform [19,20,22]:

$$c_j = -\prod_{k=1}^{j-1}(\sigma_z^k)\sigma_-^j; \qquad a_k = \sqrt{\frac{2}{N+1}}\sum_{j=1}^{N}\sin(kj)c_j,$$

where $k = \frac{\pi n}{N+1}$, $n \in$ integers. The NN coupling XY Hamiltonian is diagonal in terms of fermion operators:

$$\mathcal{H}_{\mathsf{xy}} = d\sum_j (c_j^\dagger c_{j+1} + c_j c_{j+1}^\dagger) = 2d\sum_k \cos(k) a_k^\dagger a_k. \quad (1)$$

In order to diagonalize the DQ Hamiltonian, we need a further transformation to Bogoliubov operators [23]: $a_k = \frac{1}{\sqrt{2}}(\gamma_k d_k + d_{-k}^\dagger)$, where $\gamma_k \equiv \mathrm{sgn}(k)$. We finally obtain a diagonal form,

$$\mathcal{H}_{\mathsf{dq}} = -2d\sum_k \cos k(d_k^\dagger d_k + d_{-k}^\dagger d_{-k} - 1), \quad (2)$$

with the same eigenvalues as the XY Hamiltonian.

Assuming that the polarization resides initially just on spin j, the initial state is

$$\rho_j(0) = \frac{\mathbb{1}}{2} - \frac{2}{N+1}\sum_{k,h}\sin(kj)\sin(hj)a_k^\dagger a_h,$$

which evolves under the XY Hamiltonian (1) as

$$\rho_j^{\mathsf{xy}}(t) = \frac{\mathbb{1}}{2} - \frac{2}{N+1}\sum_{k,h}\sin(kj)\sin(hj)e^{-i(\psi_k-\psi_h)t}a_k^\dagger a_h,$$

where $\psi_k(t) = 2dt\cos k$. At a time t, the polarization transferred to another spin l is given by $\mathrm{Tr}[\rho_j^{\mathsf{xy}}(t)\sigma_z^l]$,

$$P_{jl}^{\mathsf{xy}}(t) = \frac{4}{(N+1)^2}\left|\sum_k \sin(kj)\sin(kl)e^{-i\psi_k(t)}\right|^2.$$

Evolution under the DQ Hamiltonian with the same initial state yields

$$\rho_j^{\mathsf{dq}}(t) = \frac{\mathbb{1}}{2} - \frac{2}{N+1}\sum_{k,h}\sin(kj)\sin(hj)[i\sin\psi_k(t)\cos\psi_h(t) \times (a_h^\dagger a_{-k}^\dagger - a_{-k}a_h) + (\cos\psi_k(t)\cos\psi_h(t)a_k^\dagger a_h + \sin\psi_k(t)\sin\psi_h(t)a_h a_k^\dagger)]$$

and the polarization transferred to the l spin at time t is

$$P_{jl}^{\mathsf{dq}}(t) = \frac{4}{(N+1)^2}\mathrm{Re}\left[\left(\sum_k \sin(kj)\sin(kl)e^{-i\psi_k(t)}\right)^2\right],$$

where $\mathrm{Re}[\cdot]$ is the real part of a complex number. The polarization transfer is the same if the difference $b - a$ is even: $P_{jl}^{\mathsf{xy}}(t) = P_{jl}^{\mathsf{dq}}(t)$ (see Fig. 1). Even when considering a fully dipole coupled chain the difference between the

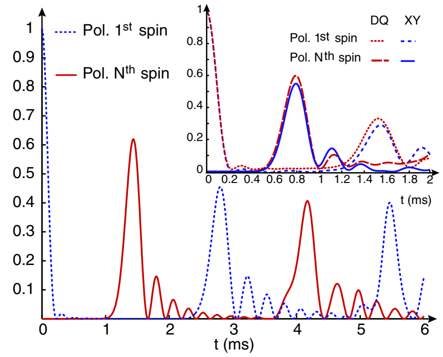

FIG. 1 (color online). Polarization transfer from spin one to spin N for a chain of 21 spins with NN coupling only; the results of evolution under double-quantum and XY Hamiltonian are superimposed. The dipolar coupling strengths considered are those found in a Fluorapatite crystal [20]. In the inset, simulations for 11 spins in a fully coupled dipolar spin chain. The differences in signal between the evolution under the full DQ and XY Hamiltonian are small for the times of interest, allowing for transport from one end of the chain to the other and back.

polarization transferred by the DQ and XY Hamiltonian remains small for the times of interest as shown in the inset of Fig. 1. In the case where the difference $l - j$ is odd, only the absolute values of the two polarization transfer are equal ($P_{jl}^{\mathrm{xy}}(t) = \| P_{jl}^{\mathrm{dq}}(t) \|$), since the observable is no longer invariant under the similarity transformation and one should have applied the transformation $U_{\mathrm{dq}}^{\mathrm{xy}}$ explicitly to recover the exact equivalence.

More generally, if we measure a different observable than σ_z^l, we expect different behaviors whether the evolution is driven by $\mathcal{H}_{\mathrm{dq}}$ or $\mathcal{H}_{\mathrm{xy}}$. In particular the XY-Hamiltonian conserves the total magnetic number (the system remains in the zero-quantum coherence manifold), while the DQ Hamiltonian can create multiple quantum coherence (MQC), states that show a coherence between different z-magnetic moment states [18]. In the NN coupling limit, the DQ Hamiltonian creates only zero and double-quantum coherences [19].

This property of the DQ Hamiltonian provides a means to detect the occurred transfer of polarization. The transport of polarization cannot be detected directly (unless one could introduce very strong magnetic field gradients or if one could perform single-spin detection). In the case of double-quantum dynamics, however, there is a correlation between the coherence intensities and the transport of the spin state, which arise from boundary effects in finite length spin chains [24].

MQC intensities can be detected in NMR, by encoding the coherence order into a phase associated with collective rotations around the z axis [18,25]. In MQC experiments, states with higher coherence orders are first prepared, for example, using $\mathcal{H}_{\mathrm{dq}}$, $\rho(0) \xrightarrow{\mathcal{H}_{\mathrm{dq}}} \rho = \sum_q \rho^{(q)}$, where q indicates the coherence order. A φ-rotation around the z axis, obtained with collective control, tags each coherence component with a phase proportional to its coherence order $\varphi(q) = q\varphi$. The system is then brought back to a single-coherence state in order to be measured, with the phases now transformed into population differences. The experiment is repeated M_q times, systematically incrementing $\varphi = 2\pi k/M_q$ ($k = 1, \ldots, M_q$), so that the signal can be Fourier-transformed with respect to it, yielding the intensity of each coherence. Restricting the interaction to nearest-neighbor only in 1D, the zero- and double-quantum intensities $J_\alpha(t) = \mathrm{Tr}[\rho^{(\alpha)}\rho^{(-\alpha)}]$ can be calculated analytically [20], yielding for an initial state with only spin j polarized

$$J_0^j(t) = \frac{4}{(N+1)^2} \sum_{k,h} \sin(kj)^2 \sin(jh)^2 \cos[\psi_k(t) + \psi_h(t)]^2,$$

$$J_2^j(t) = \frac{2}{(N+1)^2} \sum_{k,h} \sin(kj)^2 \sin(hj)^2 \sin[\psi_k(t) + \psi_h(t)]^2.$$

These intensities present a beating every time the polarization reaches spin $N + 1 - j$ and back to j. These beatings are particularly clear for the transfer from spin 1 to spin N, although they would exist for the magnetization starting at any spin in the chain. If one is therefore interested in the transfer of polarization from one end of the chain to the other, it is possible to follow the transfer driven by the DQ Hamiltonian by measuring the MQC intensities. If the measurement can only detect the total magnetization, the MQC intensities are then calculated from $\mathrm{Tr}[\rho(t)^{(-n)} \times (U_{\mathrm{dq}} \sum \sigma_z U_{\mathrm{dq}}^\dagger)^{(n)}]$, resulting in

$$\mathcal{J}_0{}^j(t) = \frac{2}{(N+1)} \sum_k \sin^2(kj)\cos^2 2\psi_k(t),$$

$$\mathcal{J}_2{}^j(t) = \frac{1}{(N+1)} \sum_k \sin^2(kj)\sin^2 2\psi_k(t),$$

and a less visible signature (as shown in Fig. 2).

It has been shown [20] that with collective coherent and incoherent control it is possible to create the initial state $\sigma_z^1 + \sigma_z^N$ (even if it is not possible to break the symmetry between the two spins at the end of the chain). In Fig. 2 we show the transport and detection method results for this particular initial state, realizable experimentally. The beating of the MQC intensities is now faster than the transfer of polarization, since the coherences start spreading out from the two opposite ends of the chain and an extremum in the MQC intensity is created when the two waves meet at the center of the chain as well as when they bounce off the boundaries. This classical interference occurs with a positive or negative phase, depending on the number (odd or even, respectively) of spins in the chain. Every two beatings, however, the maximum of the zero-quantum intensity correspond to the transport of polarization from one end to the other. This is the experimentally measurable signature that transport of polarization has occurred.

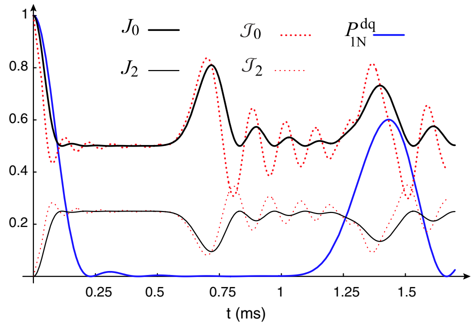

FIG. 2 (color online). MQC intensities and polarization transfer in a 21-spin chain. The initial state was the one we can prepare experimentally, $\rho_0 = \sigma_z^1 + \sigma_z^N$ [20].

An experimental study of this scheme can be implemented in single crystal of fluorapatite [7,20]. These crystals present a quasi-1D structure, where fluorine spins-1/2 are arranged in linear chains, with the cross-chain couplings much smaller than the in-chain couplings (40:1 in a particular crystal orientation). Good control, long decoherence times and the availability of the desired initial state make this system very promising. In addition, a real system will provide more insight into the limitations of the NN coupling approximation. There already exist schemes for reducing a long-distance interaction to nearest-neighbors only [26], but they are valid only for a restricted number of spins. On the other hand it is interesting to study the role of the long-range couplings in accelerating or impeding the transport. Next-nearest-neighbor couplings and cross-chain couplings offer additional pathways that can result in an acceleration of information transport, which has no classical counterpart, as already observed in the transport of dipolar energy in spin diffusion [10]. It will be interesting to investigate the differences between the predicted rate of transport and the experimental one, to observe the effects of the additional couplings on the spin dynamics.

In conclusion, we have shown how the DQ Hamiltonian simulates the transport of polarization and enables its detection. This is made possible by the observation that not only is this Hamiltonian related to the XY interaction via a similarity transformation, but it also creates coherent states, whose intensities are correlated to the transport of polarization and can be measured experimentally. With this scheme it will be possible to study experimentally, in solid state NMR systems, the transport of polarization beyond exactly solvable models and explore the appearance of quantum coherence and interference effects.

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