Transport Behavior and Dynamical Control in Integrable and Chaotic Spin-1/2 Heisenberg Chains

Lea F. Santos
Department of Physics, Yeshiva University, 245 Lexington Ave, New York, NY, 10016, USA
E-mail: lsantos2@yu.edu

Abstract. We study transport of local magnetization in spin-1/2 Heisenberg chains in integrable and chaotic regimes at zero temperature. A clean Heisenberg chain with only nearest-neighbor interactions is integrable, whereas the addition of frustrating next-nearest neighbor interactions or yet of on-site disorder may lead to the onset of chaos. For a particular initial state far from equilibrium, the dynamics of local magnetization in the chaotic and non-chaotic clean chains is surprisingly similar, but differ significantly from the disordered system. We also discuss how quantum control methods consisting of sequences of magnetic pulses may be used to remove the effects of particular terms of the Hamiltonian, such as defects or unwanted interactions, and therefore induce a desired transport behavior.

1. Introduction
Transport properties in low dimensional quantum systems are central in studies of out-of-equilibrium phenomena. Recently, the interest in the subject has been reinforced by the prospect of investigating the dynamics of strongly correlated quantum systems for long times with ultracold atoms in optical lattices [1] and by experimental results showing excess thermal conductivity in magnetic compounds [2]. Among the ongoing discussions we cite possible differences in transport properties of integrable and non-integrable models at infinite [3] and finite temperatures [4], the conditions for thermalization of isolated quantum systems [5], and the derivation of the Fourier law from a microscopic point of view [6].

In the present work, we address the more recent question concerning the transport behavior of integrable and chaotic isolated systems at zero temperature in the case of highly perturbed initial states [7, 8, 9, 10, 11]. The system considered is a spin-1/2 Heisenberg chain with open boundary conditions. We find that for a range of parameters of the system Hamiltonian, the exponent quantifying the initial decay of local magnetization in both clean chains, with only nearest-neighbor interactions (integrable) and with frustration (non-integrable), is larger than for the system with on-site disorder (chaotic), suggesting a lower scattering rate in the former cases. Contributing to this conclusion, the evolution of local magnetization in the isotropic clean chains shows a very similar bouncing behavior, which is nonexistent in the disordered system.

We also examine how appropriately designed sequences of radiofrequency (rf) magnetic pulses may be applied to control transport behavior in spin systems. This is accomplished by averaging out unwanted terms of the Hamiltonian – a method used in nuclear magnetic resonance (NMR) spectroscopy [12] and also popular in quantum information [13].
2. System Model

We consider a one-dimensional Heisenberg spin-1/2 system with open boundary conditions described by the Hamiltonian,

\[ H = H_z + H_{NN} + H_{NNN} \]

\[ = \sum_{n=1}^{L} \omega_n S_n^z + \sum_{n=1}^{L-1} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z) + \sum_{n=1}^{L-2} J'(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y + \Delta S_n^z S_{n+2}^z), \]

where \( h = 1, L \) is the number of sites, and \( S_n^{(x,y,z)} \) are the spin operators at site \( n \). The Zeeman splitting \( \omega_n \) of spin \( n \) is determined by a static magnetic field in the \( z \) direction. The system is clean when all sites have the same energy splitting, \( \omega_n = \omega \), and it is disordered when the energies differ by a value \( d_n, \omega_n = \omega + d_n \); sites with \( \omega_n \neq \omega \) are the defects. The interaction strengths \( J \) and \( J' \) of nearest-neighbor (NN) and next-nearest-neighbor (NNN) couplings, respectively, are assumed to be constant; \( \Delta \) is the anisotropy associated with the Ising interaction. We set \( J, J' > 0 \). The system is supposed to be at zero temperature and in the gapless phase, \( 0 < \Delta \leq 1 \). Under certain conditions, this model may also be mapped into systems of spinless fermions and hard-core bosons.

The total spin operator in the \( z \) direction, \( S^z = \sum_{n=1}^{L} S_n^z \), is conserved. We take \( L \) even and study the largest subspace, \( S^z = 0 \), of size \( N = L!/(L/2)!^2 \). Three systems are analyzed: (i) clean with NN coupling only \((d_n, J' = 0)\), (ii) clean and frustrated \((d_n = 0, J = J')\), (iii) disordered with a single defect and only NN interaction \((d_{L/2+1} = J/2, J' = 0)\). Model (i) is integrable [14], whereas models (ii) and (iii) are chaotic – they show a Wigner-Dyson distribution \( P_W D(sp) \) for the spacings \( sp \) of neighboring energies [15, 16]. Notice that models (i) and (ii) conserve parity, conserve total spin when \( \Delta = 1 \), and are invariant under a \( \pi \) rotation of all spins when \( S^z = 0 \). Thus, the frustrated chain can only show a Wigner-Dyson distribution if these symmetries are also taken into account [11].

The average degree of spatial delocalization of both chaotic models are comparable and 20% larger than for the integrable system. This is verified by computing the inverse participation ratio, \( \text{IPR}_j = (\sum_{k=1}^{N} |c_j^k|^4)^{-1} \), for each eigenstate \( |\psi_j\rangle = \sum_{k=1}^{N} c_j^k |\varphi^k\rangle \) of \( H \) (1) written in the basis of eigenvectors \( |\varphi^k\rangle \) of \( S^z \). A large \( \text{IPR}_j \) indicates that state \( |\psi_j\rangle \) is delocalized. In the case of \( L = 12 \) we find the following average values for \( \sum_{j=1}^{N} \text{IPR}_j/N \):

| clean+NN | clean+NN+NNN | \( d/f = J/2+NN \) |
|----------|--------------|------------------|
| \( \Delta = 1 \) | 178 | 220 | 218 |
| \( \Delta = 0.8 \) | 192 | 246 | 236 |

The dependence of the IPRs on the state energies (E) is shown in the left panels of Fig. 1. For model (iii), the curve is typical of Two-Body Random Ensembles (TBRE) [17]. It is also narrower than for the clean chains, indicating that the nearby eigenstates of the disordered system have closer degrees of complexity and localization properties.

3. System Dynamics

The right panels of Fig. 1 show the evolution of IPR for a highly perturbed initial state consisting of spins pointing up in the first half of the chain and down in the second half, \(|\Psi(0)\rangle = |1_1 \ldots 1_6 |1_7 \ldots 1_{12}\rangle\). After a quantum quench it evolves to \(|\Psi(t)\rangle = \sum_{k=1}^{N} A_k(t) |\varphi^k\rangle \) leading to changes in the level of delocalization \( \text{IPR}(t) = (\sum_{k=1}^{N} |A_k(t)|^4)^{-1} \). The behavior of the clean chains, specially at \( \Delta = 1 \), is very similar. IPR alternates between peaks of delocalization and valleys of localization, although both extremes reduce in time. The disordered system, on
system dynamics and therefore manipulate transport behavior [9, 11].

Dynamical decoupling methods consist of sequences of unitary control operations designed to average out unwanted terms of the Hamiltonian. These techniques may be used to modify the system dynamics and therefore manipulate transport behavior [9, 11].

The effects of on-site disorder, for instance, may be removed from \( H(1) \) by applying a sequence of spin echoes, that is, strong magnetic fields (pulses) that rotate all spins by \( 180^\circ \)
around a direction perpendicular to $z$. This may be accomplished with instantaneous pulses $P_x = \exp\left(-i\pi \sum_{n=1}^{L} S_n^x\right)$ repeatedly applied after every interval $\Delta t$ of free evolution. Since these pulses rotate all spins, they have no effect on the interaction terms, whereas the signs of the one-body terms are frequently alternated. After any time multiple of $2\Delta t$, the on-site energies are then averaged out in first order of $\Delta t$. As shown in Fig. 3, the disordered system then recovers the bouncing behavior of $\langle M(t) \rangle$ that was obtained with the integrable clean chain.

5. Conclusion
We studied three Heisenberg chains: clean with nearest-neighbor interactions only (integrable), clean with nearest- and next-nearest-neighbor interactions of the same magnitude (chaotic), and disordered with nearest-neighbor interactions (chaotic). For the highly perturbed initial state considered, the transport of local magnetization shows a bouncing behavior for the clean chains at $\Delta \sim 1$. The exponent quantifying the decay of local magnetization in these systems when $0.5 \leq \Delta \leq 1$ is also larger than in the disordered case. It remains to be proved if these features of the clean systems are (or not) reflecting ballistic transport. We also showed that the transport behavior of a clean system may be recovered in a system with on-site disorder by applying to it a sequence of spin echoes. Quantum control methods may therefore become useful tools to manipulate transport behavior in spin systems.

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References
[1] Paredes B and et al 2004 Nature 429 277
[2] Sologubenko A V et al 2000 Phys. Rev. Lett. 84 2714; Sologubenko A V et al 2001 Phys. Rev. B 64 054412; Hess C 2007 Eur. Phys. J. Special Topics 151 73
[3] Fabricius K and McCoy B M 1998 Phys. Rev. B 57 8340
[4] Fabricius K et al 1998 Phys. Rev. B 57 8340; Narozhny B N et al 1998 Phys. Rev. B 58 R2921; Heidrich-Meisner F et al 2003 Phys. Rev. B 68 134436
[5] Rigol M, Dunjko V and Olshanii M 2008 Nature 452 854
[6] Mejia-Monasterio C and Wichterich H 2007 Eur. Phys. J. Special Topics 151 113
[7] Gobert D, Kollath C, Schollwöck U and Schütz G 2005 Phys. Rev. E 71 036102
[8] Steinigeweg R, Gemmer J and Michel M 2006 Europhys. Lett. 75 406
[9] Santos L F 2008 Phys. Rev. E 78 031125
[10] Langer S, Heidrich-Meisner F, Gemmer J, McCulloch I P and Schollwöck U 2009 Phys. Rev. B 79 214409
[11] Santos L F 2009 J. Math. Phys. 50 095211
[12] Haeberlen U 1976 High Resolution NMR in Solids: Selective Averaging (New York: Academic Press)
[13] Santos L F and Viola L 2008 New J. Phys. 10 083009
[14] Alcaraz F C, Barber M N, Batchelor M T, Baxter R J and Quispel G R W 1987 J. Phys. A 20 6397
[15] Hsu T C and d’Auriac J C A 1993 Phys. Rev. B 47 14291
[16] Santos L F 2004 J. Phys. A 37 4723
[17] Kota V K B 2001 Phys. Rep. 347 223