Energy transport in disordered spin systems - numerical study

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Spring 2010
(Dated: May 7, 2010)

The aim of this paper is to investigate transport properties of disordered spin systems with no energy dissipation. The idea was to extend their work by analysing slightly different systems (differing mainly in the disorder factor). Investigating many systems according to the same prescription would allow for direct comparison and could result in a better understanding of how the transport properties are affected by randomness. Unfortunately, the numerical scheme fails to yield any reliable results and so the paper is dedicated mainly to analysing this issue and trying to resolve it. The main problems have been identified as lack of convergence and chaotic behaviour (especially in the low field regime). One may hope that a significant increase in computational power would resolve these problems. However, I am not aware of any mathematical reasons (or even physical intuition) to support this statement. Another way to resolve the problems is to include some dissipative modes. However, their absence was an essential assumption of the model I adopted so one would need to develop a new model to describe the transport properties in the presence of dissipative modes.

1. INTRODUCTION

Energy transport in disordered spin systems is an appealling research topic due to a couple of reasons. Firstly, the description of the problem is very simple and the numerical methods are relatively straightforward. Secondly, it is difficult to derive analytical expressions that would be valid in the long-time limit. Thirdly, numerical simulations often yield non-trivial conclusions even for simple systems. This paper focuses on the long-time behaviour of one-dimensional ring systems. The energy currents are induced by randomness in the initial conditions, local magnetic fields and coupling constants. There have been papers recently describing similar calculations which revealed interesting relations between the transport properties and different types of randomness. However, as these papers took slightly different approaches and focused on different properties it was not possible to directly compare the results. The idea of this paper was to reproduce their results in a unified way and also investigate some new systems. This would allow a direct comparison across a wide range of different systems which could contribute significantly to our understanding of the transport properties in disordered media. Also, it would be important to compare them with equivalent results in quantum spin systems (recently investigated in [1] and [2]).

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2. MODEL, TIME EVOLUTION AND TRANSPORT PROPERTIES

2.1. The model

The simplest system that exhibits continuous time evolution is the XY model ([3]). However, due to technical subtleties it is easier to consider a ring of classical Heisenberg spins (three-component unit-length vectors), $\boldsymbol{S}_k$, placed at site k (or equivalently a linear chain with periodic boundary conditions, $\boldsymbol{S}_{L+1} = \boldsymbol{S}_1$) . Each spin interacts with its nearest neighbour through a coupling of strength J_k and also with the local (time-independent) magnetic field $\boldsymbol{h}_k$. Kinetic energy is not taken into account. The Hamiltonian, H, of the system is

$$H = \sum_{k=1}^{L} (\boldsymbol{h}_k \cdot \boldsymbol{S}_k + J_k \boldsymbol{S}_k \cdot \boldsymbol{S}_{k+1}) \tag{1}$$

If we define the effective local magnetic field as

$$\boldsymbol{H}_k = \frac{\partial H}{\partial \boldsymbol{S}_k} = \boldsymbol{h}_k + J_k \boldsymbol{S}_{k+1} + J_{k-1} \boldsymbol{S}_{k-1} \tag{2}$$

then the equations of motion are

$$\frac{\partial \boldsymbol{S}_k}{\partial t} = \boldsymbol{H}_k \times \boldsymbol{S}_k \tag{3}$$

The initial orientation of each spin is drawn from a uniform distribution of unit vectors. The details of how $\boldsymbol{h}_k$ and J_k are generated are described in the next section. In order to investigate transport properties of this system it is essential that the total energy is conserved (to numerical precision). We do so by letting the even-numbered spins precess while the odd-numbered are stationary and then vice versa in the next time step. This method and its implications are thoroughly discussed in [4] and the conclusion is that although this change of dynamics is significant, it should not affect the qualitative, long-time,

low-frequency behaviour that we aim to investigate in this paper.

2.2. Transport properties

We start by defining the local energy $e_k(t)$ at site k

$$e_k(t) = \boldsymbol{h}_k \cdot \boldsymbol{S}_k + \frac{1}{2}(J_{k-1}\boldsymbol{S}_{k-1} \cdot \boldsymbol{S}_k + J_k \boldsymbol{S}_k \cdot \boldsymbol{S}_{k+1}) \quad (4)$$

Note that this definition splits the interaction energy equally between both sites which leads to a straightforward and unambigous definition of the energy current at site k. However, because of the asymmetry between the even- and odd-numbered spins (the even-numbered precess first) the expressions for odd and even k are slightly different. For even k

$$j_k(t) = [\boldsymbol{S}_k(t+1) - \boldsymbol{S}_k(t)] \cdot [J_k \boldsymbol{S}_{k+1}(t) - J_{k-1}\boldsymbol{S}_{k-1}(t)] \quad (5)$$

while for odd k

$$j_k(t) = [\boldsymbol{S}_k(t+1) - \boldsymbol{S}_k(t)] \cdot [J_k \boldsymbol{S}_{k+1}(t+1) - J_{k-1}\boldsymbol{S}_{k-1}(t+1)] \quad (6)$$

The assumption that each instance of the system has the same Boltzmann weight (regardless of its energy) corresponds to infinite temperature ($\beta = 0$). Therefore, the conventional thermal conductivity vanishes. Instead, we use the definition of the DC thermal conductivity derived in [4] and its relation to the energy current

$$\kappa = \lim_{L,t\to\infty} \kappa_{L,t} \quad (7)$$

where

$$\kappa_{L,t} = \frac{1}{Lt}[\langle \{ \sum_{\tau=1}^{t} \sum_{k=1}^{L} j_k(\tau) \}^2 \rangle] \quad (8)$$

The computation of κ comprises, therefore, of 2 parts. First, by averaging over many initial conditions an estimate of $\kappa_{L,t}$ is calculated for fixed values of L, t and then many of these estimates are required to converge in the limits $L, t \to \infty$ to yield the final value of κ.

2.3. Random variables

The two random variables in our system are $\boldsymbol{h}_k$ and J_k. The local magnetic fields - $\boldsymbol{h}_k = \boldsymbol{h}_k = h_k \hat{\boldsymbol{n}}_k$, are chosen such that their orientation is drawn from a uniform distribution of unit vectors (similarly to the initial conditions), whereas the strength is drawn from a Gaussian distribution characterised by mean zero and variance Δ^2. Note that the case $\Delta^2 = 0$ corresponds to zero magnetic field. The distributions of J_k that we want to investigate are:

1. J_k drawn from a uniform distribution in the interval $[J_0(1-\epsilon), J_0(1+\epsilon)]$; the first two moments of this distribution are $\langle J \rangle = J_0$ and $\langle J^2 \rangle = J_0^2(1 + \frac{\epsilon^2}{3})$. Note that for $\epsilon = 0$ this is exactly the case investigated in [4]. The case for $\epsilon > 0$ was studied in [5], however without any magnetic fields.

2. J_k drawn from a normal distribution centred at J_0 with variance σ^2

3. J_k drawn from a binomial distribution such that $J_k = J_0$ with probability p and $J_k = \lambda J_0$ otherwise. Positive λ would correspond to having two distinct types of bonds (strong and weak). In this case one may expect that the overall conductivity will be limited by the weakest link. Negative λ would correspond to having some antiferromagnetic bonds in the system and one may expect that such interactions should decrease the conductivity.

2.4. Numerical scheme

As in every numerical study the compromise between precision and capability of reaching long timescales is difficult. The basic unit of the computation is evolving a single instance of the system. This is done by discrete time-step evolution until one of the two following events occurs:

1. the relative error in the total energy exceeds some fixed value
   This indicates that numerical errors have built up and we should no longer trust the calculation. We reduce the time step and start the evolution from the beginning (same initial conditions). Initially I performed the evolution step in Cartesian coordinates because the equations were more straightforward to code. However, then I had to check that the length of each spin is preserved at all times. This issue can be eliminated by switching to spherical polar coordinates and fixing the length explicitly (appendix A includes the relevant equations).

2. the conductivity converges
   For convergence we require that during the last interval of the evolution (defined as a fixed fraction f of the total time t) fluctations of conductivity do not exceed some fraction α of the final value. Formally this condition can be written as

$$\forall \tau \text{ such that } (1-f)t \leq \tau \leq t, \quad |\frac{\kappa(\tau) - \kappa(t)}{\kappa(t)}| \leq \alpha \quad (9)$$

Assuming that the conductivity converges, the scheme above gives a way of finding it to arbitrary precision provided we have unlimited computational power. Next step is to take the average over many instances of the system and then find the limits as $L, t \to \infty$. In order to ensure

that these operations have been done correctly one needs a large set of data points which makes the computation rather expensive.

3. RESULTS

Unfortunately, the scheme presented above exhibits very unstable behaviour. The two main issues are lack of convergence and chaotic behaviour. The first one means that I cannot obtain required level of convergence using available computational resources, whereas the second one means that even if I obtained some convergent results they should be treated with care as the model exhibits some chaotic features.

3.1. Lack of convergence

The convergence depends strongly on the initial conditions and in a significant fraction of cases it is prohibitively slow. In order to investigate these problems I tried to reproduce exactly the calculation from [4] which corresponds to $J_0 = 0.5$, $\Delta^2 = 0.5$ and $\epsilon = 0$. The following figure shows the usual issues arising during the simulation. We have generated a particular instance of the system, all the random initial conditions have been chosen. Now we need to evolve it and adopting weak convergence conditions ($f = 0.1$, $\alpha = 0.02$) yields some limit (Fig. 1). I am aware that these conditions are so weak that the limit should not be trusted at all but I have not managed to obtain any better convergence. In order to check whether this is a true convergence or just a local plateu we run the same simulation with more stringent convergence conditions ($f = 0.2$) and the conclusion is that the previously encountered convergence was purely accidental (Fig. 2). Actually, it turns out that under these stronger conditions the conductivity does not converge even for significantly longer times (Fig. 3). This example shows the most severe and common problem I have encountered: we can obtain some limits for weak convergence conditions but on making them more stringent all these limits turn out to be accidental and even long time evolution does not lead to convergence (I have run multiple simulations up to 20 hours long and I have not managed to converge a single instance for $f = 0.2$, $\alpha = 0.02$). Clearly, in this implementation the convergence is too slow for a feasible calculation of transport properties (recall that we need to average over many instances and then take two limits). I have also tried analysing the graph in the Fourier space which yielded a continuum of low frequency modes.

When I realised that I was not able to achieve strong convergence I decided the investigate the weak convergence in the zero-magnetic field case ($J_0 = 1$, $\Delta^2 = 0$, $\epsilon = 0$). It turns out that for $f = 0.1$, $\alpha = 0.02$ and the maximum convergence time of one hour the system will either converge within 60 secs or not converge at all.

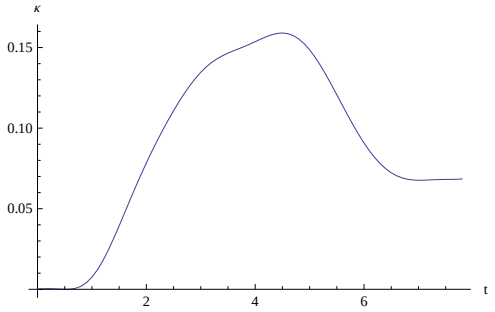

FIG. 1: The evolution under weak convergence conditions quickly results in apparent convergence.

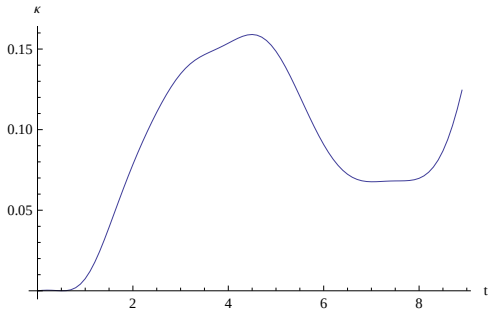

FIG. 2: More restrictive convergence conditions reveal that the previous result was purely accidental.

I have not encountered a single system that would not fall into one of the two categories. The result of this experiment are conductivities for 7893 instances. The histogram of the time (in arbitrary units) necessary for convergence is presented in Fig. 4.

The conductivities for this set of results follow approximately a normal distribution with $\kappa_0 = -0.011$ and $\sigma = 2.172$ (Fig. 5).

In order to check whether averaging over many instances leads to convergence I calculated the average of the first n points and plotted it for $1 \leq n \leq 7893$ (Fig. 6). Unfortunately the result is a curve that seems to exhibit fluctuations at all scales and concluding any convergent features from this data set would be at best suggestive.

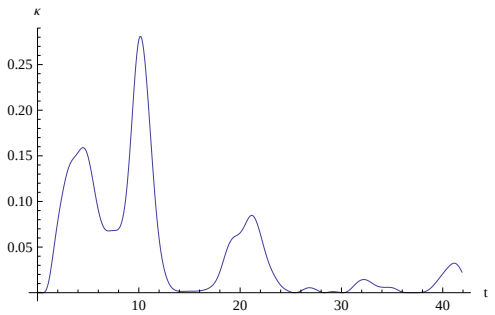

FIG. 3: Even significantly longer time evolution does not lead to convergence under stronger convergence conditions.

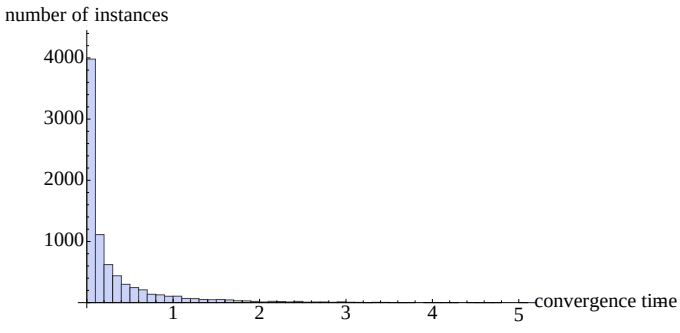

FIG. 4: Histogram of convergence times.

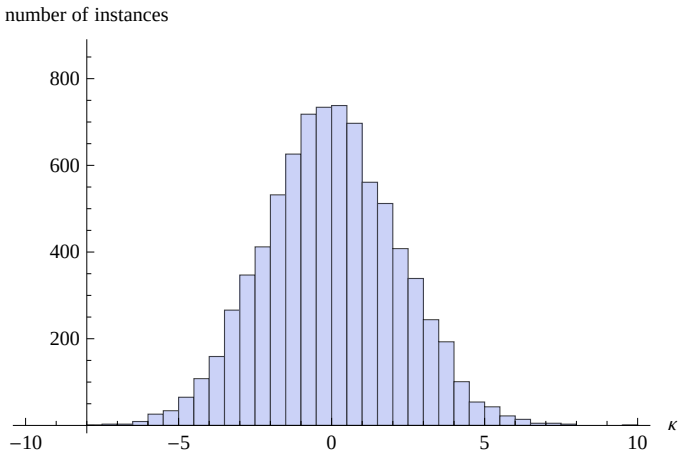

FIG. 5: Histogram of conductivities.

3.2. Chaotic behaviour

When the program realises that the numerical precision has been lost it reduces the time step and restarts the same simulation. I would expect that the second curve will follow the first one closely. However, there are situations when reducing the time step changes the character of the curve drastically (this seems to be especially common for low magnetic fields). Below I present two examples of this behaviour for $J_0 = 0.6$, $\Delta^2 = 0.28$, $\epsilon = 0$ (Fig. 7) and $J_0 = 1$, $\Delta^2 = 0$, $\epsilon = 0$ (Fig. 8), respectively. For small times all curves are very similar but as the time elapses they start to separate. Clearly, changing the time step may completely change the character of the curve in this regime. Unfortunately, this implies that unless we are able to explain this behaviour analytically and find some time step threshold that avoids it, there is no guarantee that our results are close to the exact solution. Also, from Fig. 7 we see that the three curves do not seem to tend to a common limit. I would even say that the first and third ones share more features than any of them with the second one.

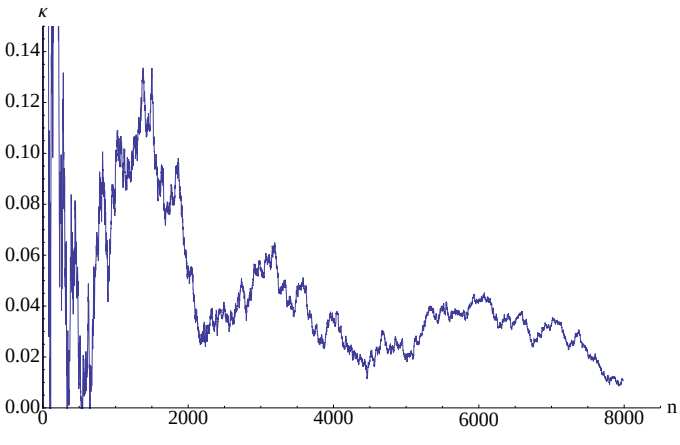

FIG. 6: Average over the first n data points.

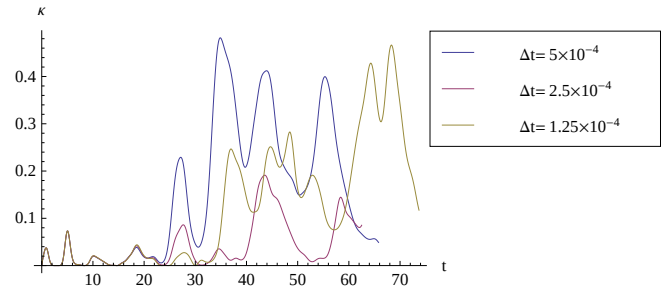

FIG. 7: Time evolution for different time steps under low magnetic field.

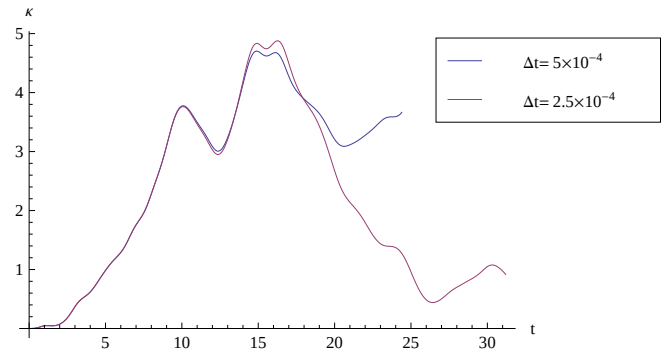

FIG. 8: Time evolution for different time steps under no magnetic field.

4. SUMMARY

Unfortunately, the whole project failed at a very early stage. I have identified the ways in which it fails and I am afraid that they may be intrinsic properties of the system. We deal with a highly disordered system with no modes of energy dissipation. Therefore, the equilibration process may be very slow up to a point where it can no longer be captured by numerical simulations (unless we have access to extremely powerful computers). An obvious solution to facilitate reaching the equilibrium state

would be to include some dissipative modes. However, this would be completely incompatible with the model I adopted (which relied on the energy conservation as the basic assumption) and so a new model would need to be developed. I have contacted the authors of [4] asking for some advice but I did not receive anything that would help me resolve my problems.

Acknowledgments

I would like to thank J. Rahi and M. Kardar for useful discussions.

Appendix A: Time evolution in spherical coordinates

The time evolution is expressed by

$$\frac{\partial \boldsymbol{S}}{\partial t} = \boldsymbol{H} \times \boldsymbol{S} \tag{A1}$$

where

$$\boldsymbol{S} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} \qquad \boldsymbol{H} = \begin{pmatrix} H_x \\ H_y \\ H_z \end{pmatrix} \tag{A2}$$

The local magnetic field ($\boldsymbol{H}$) is expressed in Cartesian coordinates whereas the spin orientation ($\boldsymbol{S}$) is expressed in spherical polar coordinates (which allows us to constrain its length to unity). Evaluating both sides yields:

$$\begin{aligned} \begin{pmatrix} \cos\theta\cos\phi\,\dot\theta - \sin\theta\sin\phi\,\dot\phi \\ \cos\theta\sin\phi\,\dot\theta + \sin\theta\cos\phi\,\dot\phi \\ -\sin\theta\,\dot\theta \end{pmatrix} = \\ = \begin{pmatrix} H_y\cos\theta - H_z\sin\theta\sin\phi \\ H_z\sin\theta\cos\phi - H_x\cos\theta \\ H_x\sin\theta\sin\phi - H_y\sin\theta\cos\phi \end{pmatrix} \end{aligned} \tag{A3}$$

which leads to the following equations of motion

$$\dot\theta = H_y\cos\phi - H_x\sin\phi \tag{A4}$$

$$\dot\phi = H_z - H_y\frac{\sin\phi}{\tan\theta} - H_x\frac{\cos\phi}{\tan\theta} \tag{A5}$$

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