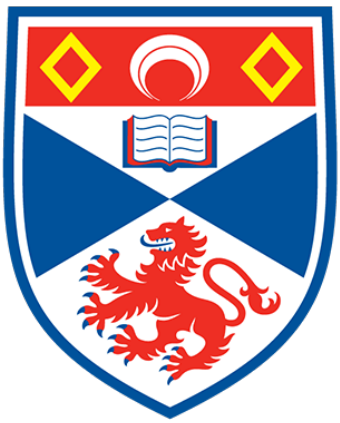
Modelling Subdiffusive Transport in Classical Disordered Systems



University of
St Andrews

NURI MORAD

Contact: nm240@st-andrews.ac.uk
Supervisor: Dr Chris Hooley
August 2023

Abstract

Quantum computation has the potential to utterly revolutionise all aspects of modern life. From weather forecasting to drug development and from AI to cryptography, many processes that today are powered by classical computation will be made exponentially faster by the development of quantum computers.
This research project set out to explore an area of theoretical physics that has potential for use in quantum computing. Many-body localised (MBL) systems' property of self-assembly could make the preparation of qubits in quantum circuit design far easier.
MBL occurs at the limit where the transport exponent of the transport of information in a given system goes to zero. Currently, we don't yet have a rigorous theoretical framework for the mechanism behind MBL. As we can only probe the phenomenon numerically, and numerical simulations become impossible when subdiffusive transport becomes extremely slow, the boundary between subdiffusive transport and true localisation, if it exists, is not yet understood.

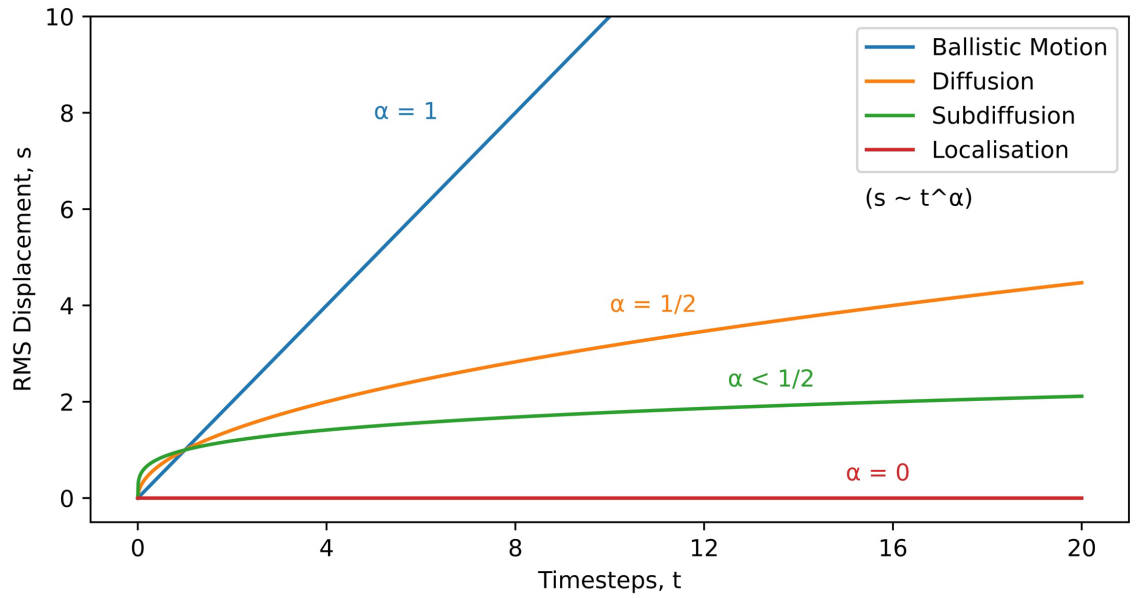


Figure 1: Graph showing different types of motion and how they relate to the transport exponent, α. Ballistic motion occurs at α = 1, diffusion at α = ½, sub-diffusion at α < ½, and MBL: α = 0.

Background

The random walker: Imagine you are standing on the centre-spot of a football pitch, and repeatedly toss a fair coin. Every time the coin lands on heads you take a step towards the goal on your left; for tails, your right. This is the most basic model for a random walk. Where might you expect to be after a given number of tosses, n (or equally, if you're tossing at a regular frequency, time)? You'll find that your root mean square (RMS) displacement - or in other words, the region either side of the centre that you expect to have 'explored' - will scale with the square-root of n. This is an example of diffusion: where the transport exponent, α (see Figure 1), is ½.
In this project, a slightly different species of random walk was examined computationally to test whether the addition of disorder – where energy is now required to make a step left or right – might cause the motion to become subdiffusive (α < ½) rather than diffusive.

Subdiffusion and the link to MBL

MBL occurs at the limit where α goes to zero. The region immediately above this is subdiffusion, so it is reasonable to expect that for a system to become localised, it must first pass through this subdiffusive phase. Understanding the behaviour of these systems as α approaches zero is analogous to understanding what causes them to become localised.
We know, from previous numerical work done in this field, that there are clean (that is, zero disorder: W = 0) classical models (an example of which being the simple random walker described above) that show subdiffusion, and disordered quantum models that do. The question we'd like to answer is whether there's a link between the origins of subdiffusion in these 2 cases. The obvious middle ground, a classical disordered system, seems a sensible to look – not least because we at least ought to know as much as we can about the behaviour of both clean and disordered classical models (in terms of showing subdiffusion) before we really have a chance at working out how to analyse the quantum ones. Moreover, the advantage of a classical model is you can actually get inside it, look at the configuration and make maps of how it evolves with time. We could thus maybe get some sense as to how it looks different in the subdiffusive phase.

From current numerics, this is the picture we have:

- In a perfectly clean system (W = 0), we often see ballistic motion – so the transport exponent, α, is 1.
- As soon as any disorder (non-zero W) is applied, α drops to ½, which is the diffusive exponent. And then it seems to stay at ½, until some first critical strength of the disorder, where it seems to drop slightly, although the numerics are not 100% clear.
- Beyond this point, you need longer and longer systems and longer and longer times to distinguish subdiffusion from localization as this subdiffusion exponent gets smaller, and so the numerics start freezing because of the finite system size. This leaves 3 different possibilities for what occurs next:
    1. Scenario 1 is that α might keep decreasing forever, approaching zero but never reaching it. In other words the sub diffusion just gets slower and slower, but never reaches true localisation (or only does at infinite disorder, which in practise is impossible). Verdict: MBL is not possible.
    2. Scenario two is that α hits zero at some second critical disorder strength, and then beyond that you have proper MBL.
    3. Scenario three is that α follows a similar trajectory but at some point jumps down to zero, and again we have proper MBL.

- With the current state of numerics on spin chains, we don't really know which of these is happening. In the specific case of the transverse field Ising chain, we have the proof by Inbri that there is an MBL phase and so it must be scenario 2 or 3. But in other spin chains we have no proof of an MBL phase, so it could also be scenario 1.

There are two ways we can attack this problem:
- One is to ask: can we start at the high disorder end and prove that MBL survives?
- The other would be to ask: can we start at the low disorder end and prove that subdiffusion can't go on forever? Because if subdiffusion can't go on forever, the only alternative presumably is MBL. If we can understand subdiffusion more generally, perhaps we can understand when that exponent has to go to zero.

Subdiffusion can also be seen in clean systems with added conservation laws. For example, a previously diffusive model plus some constraints can become subdiffusive. This is interesting because in the disordered systems, we don't know what's causing subdiffusion, but in the clean systems, it seems to be constraints that are forcing subdiffusion. This raises the idea that perhaps what's important about these constraints is that they prevent single particle hopping and instead force a move to multi particle hopping. This will naturally be less frequent than the single particle kind as it

requires greater correlation, and so that slows down the transport. It might be that the origin of the subdiffusion in the disordered spin chains is the same: that as the disorder strength increases, it gets harder to find a single particle move. It also follows that perhaps if two-particle hopping takes over from one particle hopping at some disorder strength, then maybe three particle takes over from two particle at some point, then four from three, and so on. Then perhaps there's some disorder strength at which that number of particles goes to infinity, and at that point it will become localized. The idea here again is to show that MBL takes over from subdiffusion at some finite W.

Motivation

Unlike classical systems, a quantum system cannot usually be kept in the same place (or state) indefinitely. To give the example of a particle trapped in a deep well, this is due to quantum systems' intrinsic property that there will always be a finite probability of the particle 'tunnelling' out of the well, irrespective of its depth. MBL is a phenomenon whereby tunnelling is prevented by quantum interference between the different paths by which it could happen. An MBL system then, as far as we understand, stays where you put it forever. This offers the only known possible route to keep a quantum system in a certain state indefinitely.
This property has potential applications in quantum computing, in the self-assembly of qubits. The idea of self-assembly is that you could take a spin chain, make a large random disorder, and qubits would just form. Because in the regions where the disorder happens to be large and negative, you get a region where the spin is stuck downwards, and vice versa. So, a many-body localised system exposed to some certain random disorder could self-assemble to form qubits, saving painstaking effort.
Qubits made this way would differ slightly from the current norm: Typically, the information is encoded in the qubits' spin, which in that case is in a superposition state (crucial to the function of the qubit). In this case the spins are definite by design, so the information would instead be encoded in the relative complex phases of the qubits, which can still exist in a superposition state.

This research is however (and as if often the case in science), in many ways a gamble. That is because there is only one rigorous proof of a single type of spin chain that actually shows MBL, and that proof does not establish the disorder strength that you need to cause it to happen - it only proves that it's not infinite. We have no proof for MBL occurring in any other spin chain. (We have numerical evidence that points to MBL in other scenarios, but no proof.) This of course leaves us with no guarantee of finding anything.
Another problem is that most of our current data is from numerics, which never leaves you with a complete picture. Thus the evidence we have pointing to MBL needs to be treated with caution because things tend to look localised on small scales, as it's possible they can't yet find the thing they would have tunnelled into. For example, say you have a frog on a surface of a pond, hopping between lily pads. If you limit the pond so there's only one lily pad, it looks localised, but you've actually just made the pond so small that you can't see the delocalisation processes. This is the issue when doing numerical work - you have to do it on finite size systems because computers are finite.

The Model

Before diving into the algorithm, it's worth making clear a few basic principles that guided how it was designed:

- Simulations become slower as α approaches zero, so it is impossible to do numerics for the (possible) boundary between subdiffusion and MBL.
- Nearest-neighbour swaps (of magnetisation) mediate the of transport information along spin chains.

- Transitions (or nearest-neighbour swaps) are more likely to occur at neighbouring sites whose energy differences are small.
- At larger W (larger disorder), the average energy differences become such that transitions decrease in frequency. There should thus be some transition to localisation (from subdiffusion) at large W.
- Clearly, at infinite W, the system should definitely be localised. However the statement of MBL is that the system remains localised even at finite W. It's the surprising robustness of the localized state that happens at large disorder.

Explaining the Algorithm (see Figure 2):

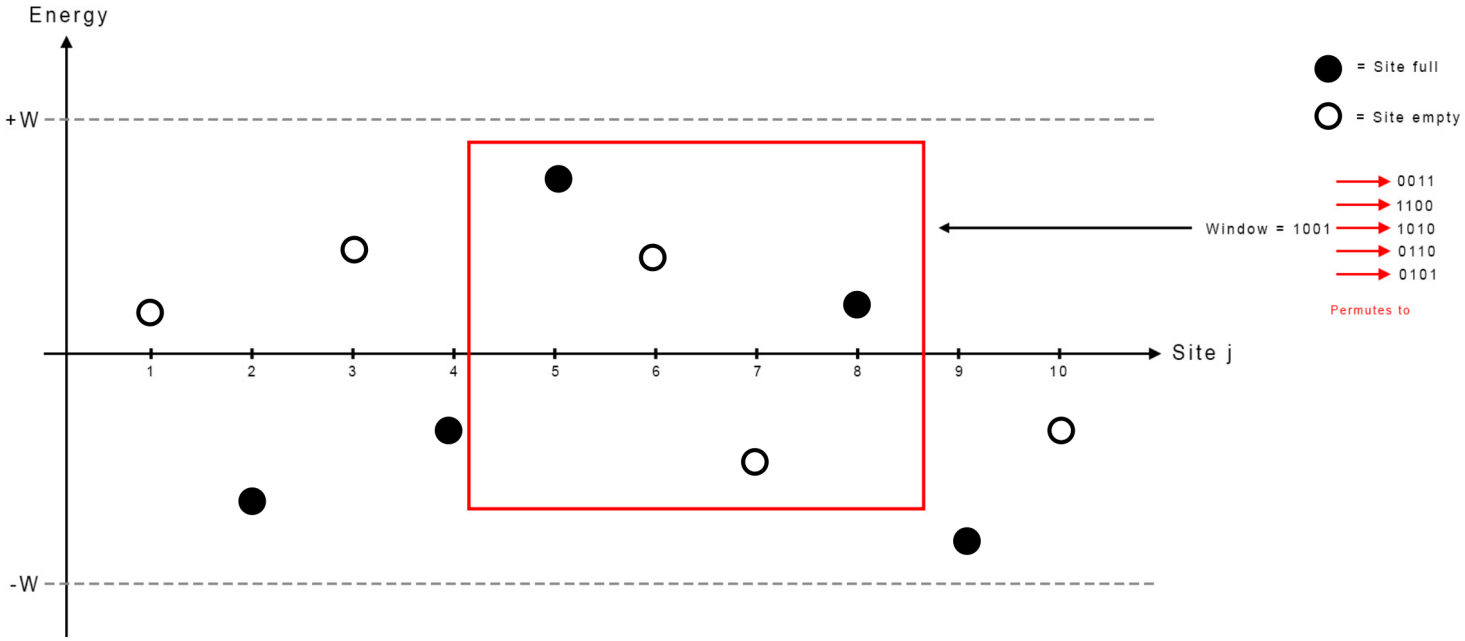


Figure 2: Diagram illustrating the action of the n-site permutation gate (in this case, 4-site), applied at a random site *j* (in this case, site 5). The occupation of the sites is represented by a binary string, where 1 = occupied site and 0 = unoccupied site. The more generic energy scale, between +W and –W, is analogous to height between 0 and 2m above the ground.

- The dynamic we simulated is similar in principle but different in mechanism to the simple random walker described above. Imagine that in place of the football pitch we now have, say, 100 baskets (or 'sites') in a line, of which half are occupied at random with a tennis ball and the other half empty. Now, place each basket at a random height between 0 and 2m above the ground.

- Instead of the coin-toss, we now apply an n-site permutation gate at a random site along the chain, which simply shuffles the tennis within that window into a new configuration.

- Finally, the permutation is accepted if the combined heights of the newly occupied baskets fall within an arbitrary height parameter, delta, of the pre-shuffled total, and rejected otherwise.

- This process is repeated at every site along the chain, in a random order.

The Δ parameter:

The Δ cut-off is designed to mimic in a rough way that in quantum mechanics you're more likely to get tunnelling between neighbouring states that are close in energy than you are to get tunnelling between neighbouring states that are far away in energy. Or in other words, you're more likely to see tunnelling through a small energy barrier than a large one.
In a classical model there can't be that fuzziness – given a certain energy gap the perturbation must either occur or not – and so instead the Δ parameter exists as a hard cut-off.
The idea is that this clearly has a Δ to infinity limit, which is diffusive, because then the particles are basically just independently random walking and so presumably you get diffusion all the time. It clearly has a limit which is localised, because if Δ equals zero, no moves are ever accepted, because the chance of any of these energies being precisely the same is mathematically zero. So it's clearly localized at Δ equals zero, it's clearly diffusive as Δ goes to infinity. So we were wondering whether, in between the localisation at small Δ and the diffusion at large Δ, there might be a sub-diffusive regime.

The autocorrelator is a measure of: if a particle is present on site j at time 0, how likely is it still to be there (where it started) at time t? If the system is localised, this number will still be non-zero even at very long times, because the particle will usually be bouncing around in some small region. For example, if the particle delocalises over five sites around where it started, but can't get any further than that, then the autocorrelator will be roughly a fifth (ie it goes as 1/localisation length). In a finite chain length the most the particle can delocalize is spreading over the length of the chain. Therefore the maximum possible localisation length = the chain length, and the autocorrelator can never be zero as its lower limit is 1/chain length.
In this way, using different chain lengths, we can test for (true) localisation by observing whether the system localises at lengths shorter than the chain length or not. We can test for diffusion/subdiffusion by plotting the log of the autocorrelator vs log of time. Seeing as their relationship is a power law, this will show up as a straight line on the plot, whose gradient will be = - α.

This model we believe to be diffusive for $\Delta > W/2$ and localised for $\Delta < W/2$.
We don't believe this model to be subdiffusive, and the suspicion is that this is due to having a fixed gate length. This is because there will probably be features in the energy landscape that are impassable for the given gate length, but that could be overcome by a longer gate. The next step therefore could be to randomly draw the gate length at each iteration from a certain distribution, which would avoid the complete localisation currently seen. It is a question of which distribution to use, but the hope/expectation is that this may show subdiffusion.
If there is a finite number of these impassable features, that guarantees you can't have diffusion because diffusion requires the particle to be able to keep on spreading out.

Next Steps

The algorithm was coded from scratch using Python, and preliminary autocorrelator graphs (such as in Figure 3) generated to confirm the model worked as expected.
It was later translated into C++ to improve runtime and to allow for running on larger clusters in the future for higher resolution data. The next step will be to examine the model using randomised variable-length gates, which is where we hope to see subdiffusion, rather than the fixed gate lengths used thus far.

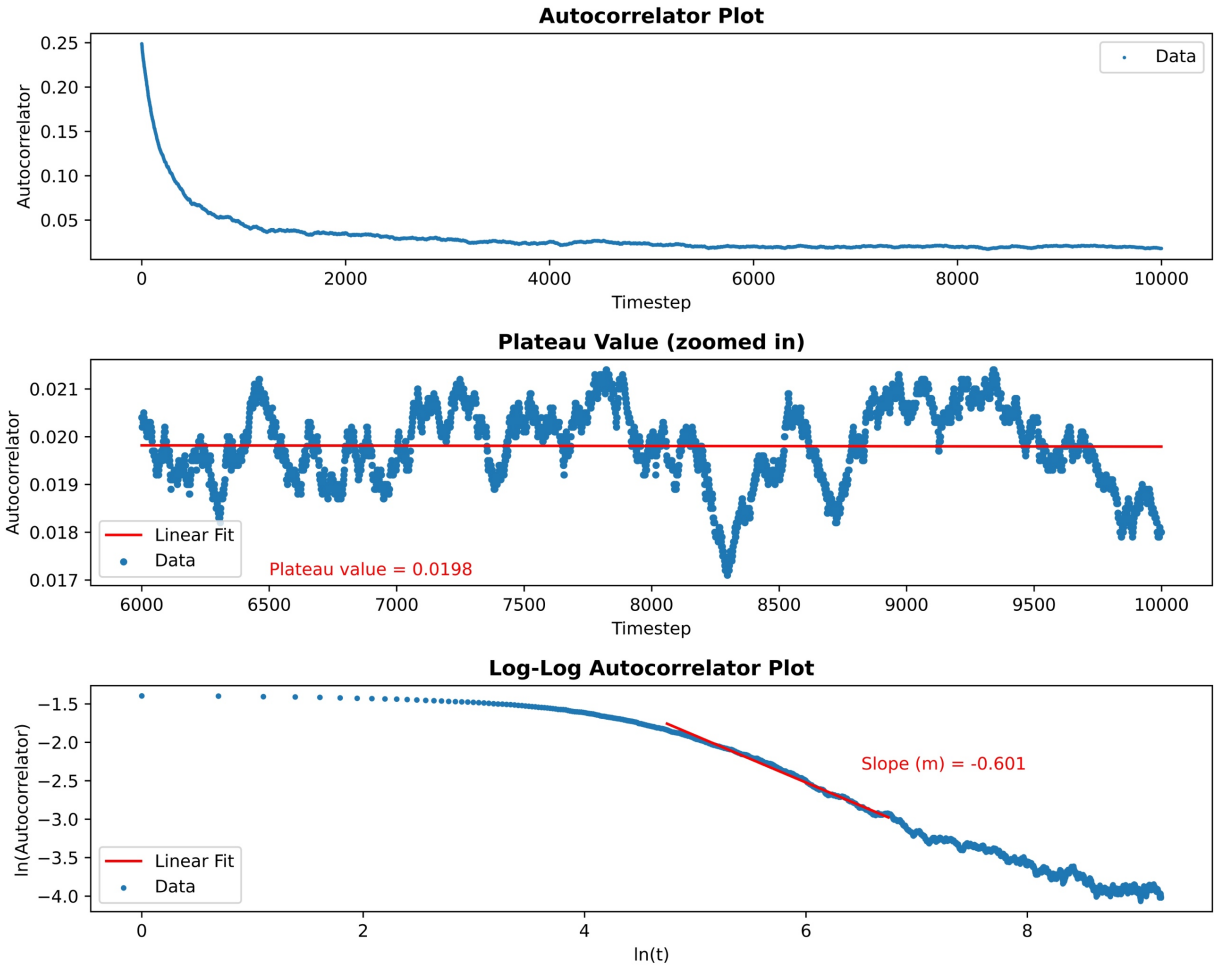


Figure 3: Some data analysis on autocorrelator values run to 10,000 timesteps at $\Delta = 0.1W$: The top graph shows the entire set of values, of which the last 4,000 are seen more closely below, and a linear fit used to establish the plateau value. The lower graph is a log-log plot of all the values, with a fit used to measure the gradient of the linear section. The noise at the bottom-right corner is an artefact of log-log graphs and ignored.

References:

1. Wang, H., Yeh, HC. & Kamenev, A. Many-body localization enables iterative quantum optimization. *Nat Commun* **13**, 5503 (2022). https://doi.org/10.1038/s41467-022-33179-y
2. Jae-yoon Choi et al. ,Exploring the many-body localization transition in two dimensions.Science352,1547-1552(2016).DOI:10.1126/science.aaf8834
3. Schulz, M. *et al.* (2018) *Energy Transport in a disordered spin chain with broken U(1) symmetry: Diffusion, subdiffusion, and many-body localization*, *Physical Review B*. Available at: https://journals.aps.org/prb/abstract/10.1103/PhysRevB.98.180201 (Accessed: 01 September 2023).
4. Singh, H. *et al.* (2021) *Subdiffusion and many-body quantum chaos with kinetic constraints*, *Physical Review Letters*. Available at: https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.127.230602 (Accessed: 01 September 2023).
5. Xia, W., Zou, J., Qiu, X. et al. The reservoir learning power across quantum many-body localization transition. Front. Phys. 17, 33506 (2022). https://doi.org/10.1007/s11467-022-1158-1
6. *Quantum Information Processing* (no date) *Yao Group*. Available at: https://quantumoptics.physics.berkeley.edu/quantum-information (Accessed: 01 September 2023).