

abstract

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Part I

Research Proposal

Chapter 1

Introduction

Chapter 2

Objectives

2.1 Assymetric VRH

If the sites have different potentials, then the site occupation probabilities change. This can be accommodated for by modifying the transition rates by Boltzmann's factor. This is called *VRH- Variable Range Hopping*[?], and has been widely studied. The common practice is to treat the system as a symmetric resistor network, but we want to ask if there are cases where this reduction to a symmetrical network is not valid.

2.2 Stotland's errata model

2.3 Geometrical implications

The geometric properties of the system are reflected in the statistics of the distances, and by extension in the statistics of the transition rates. However, there is more information in the W_{nm} matrix than just its statistics. The question arises: Are the statistics all that is needed to understand the physics of the system? See the preliminary results for farther discussion ??.

2.4 Banded sparse matrices

The conductance of quasi-1d banded sparse matrices was studied numerically in [?]. There, they use *Variable-Range-Hopping* in the sparse regime, where $(\text{sparsity} \cdot \text{bandwidth}) \ll 1$. However, in this work it is not clear what are the limits on either sparsity or bandwidth, and in particular where is the cross between the validity regime of VRH and that of SLRT. We will try to understand this issue analytically.

2.5 Diffusion or Subdiffusion in $2d$

The question of diffusion in most 1d systems was analytically solved in [?]. The $2d$ case is, as far as we know, not yet analytically solved, and is much less clear. In [?] it is claimed that in low density systems subdiffusion of order $\sim \log^d$ should occur. We wish to use the block-renormalization-group method to find out if this is indeed the case. We also wish to see if there is a transition between low densities and high densities.

2.6 The spectral properties of Sinai diffusion in $1d$

In a symmetric random rate system, there is regular diffusion if the harmonic average is bounded, i.e. if

$$\sum_n \frac{1}{w_n} < \infty$$

On the other hand, for an asymmetric system, an activation energy builds up, and a Sinai diffusion behaviour is followed. The conductance is exponentially small in the length, and the spreading is anomalous. The difference between those two models is clearly highly significant. We wish to investigate the difference between the models, and the relation of this difference to the spectral properties of the model.

2.7 Sinai diffusion in $2d$

The spectral properties, and spreading behaviour of a $2d$ asymmetric system.

2.8 The charge carrier discreteness

Our work so far considered probability rate equations, which are valid for a single particle in the network. If we have multiple interacting particles in the network, additional factors may contribute. For example, a single occupancy rule (i.e. each site may have up to one particle) may cause Fermi blocking.

2.9 Banded Random Matrices

Chapter 3

Background

3.1 Transition matrices

Our system is a d -dimensional network, and it is described by its nodes and edges. The nodes represent either *sites* in real space or *levels* in energy space, and our particle (or particles, see 2.8) may occupy them. The edges of the network represent transition rates between the nodes. The dynamics of the model are described by a rate equation:

$$\frac{dp_n}{dt} = \sum_m w_{nm} p_m$$

Where the transition matrix

$$\mathbf{W} = [w_{nm}]_{N \times N}$$

Is the crux of this work.

Because of conservation of probability, we set the diagonal elements to

$$w_{nn} = - \sum_{m(\neq n)} w_{mn}$$

3.2 Definition of the model

The proposal regards a spatial network where each node has a defined location x_n . The transition rates w_{nm} are constructed by the expression

$$w_{nm} = w_0 e^{-\epsilon_{nm}} B(x_n - x_m) \tag{3.1}$$

where $B(r)$ describes the dependence of the coupling on the distance between sites, and ϵ represent activation energies required for a transition.

The $b(r)$ matrix is a function a euclidean distance matrix, a class a matrices that is widely researched TODO

3.2.1 The random site hopping model

For presentation purpose we regard the nodes of the network as *sites*, each having a location x_n . In particular (but not exclusively) we are interested in a model where the rates depend exponentially on the distance between randomly distributed sites, namely $w_{nm} \propto \exp(|x_n - x_m|/\xi)$. One can characterize such a system by a sparsity parameter s that reflects the connectivity of the network. For a random site model the natural definition is $s = \xi/r_0$, where r_0 is the average distance between neighboring sites.

The models that we address are related and motivated by various physical problems, for example: phonon propagation in disordered solids [? ? ?]; Mott hopping conductance [? ? ? ? ?]; transport in oil reservoirs [? ?]; conductance of ballistic rings [?]; and energy absorption by trapped atoms [?]. Optionally these models can be fabricated by combining oscillators: say mechanical springs or electrical RC elements.

3.3 The study of networks

In all these examples the issue is to understand how the *transport* is affected by the *sparsity* of a network. If the rates are induced by a driving source, this issue can be phrased as going *beyond* the familiar framework of Linear Response Theory (LRT), as explained below.

3.4 Diffusion

Our interest is focused on the diffusion coefficient D that characterizes the long time dynamics of a spreading distribution. It can be defined or deduced either from the variance $S(t) \sim Dt$ or from the decay of the survival probability $\mathcal{P}(t) \sim (Dt)^{-d/2}$. Hence it is related to the spectral properties of the transition rate matrix

$$\mathbf{w} = \{w_{nm}\} \tag{3.2}$$

Exploiting the formal analogy with a resistor network calculation [?], namely w_{nm} are like connectors and D is like conductivity, one realizes that D is given by a semi-linear functional $D[\mathbf{w}]$ that has the property $D[\lambda\mathbf{w}] = \lambda D[\mathbf{w}]$, while in general $D[\mathbf{w}^a + \mathbf{w}^b] > D[\mathbf{w}^a] + D[\mathbf{w}^b]$ instead of equality.

3.5 Subdiffusion

In the 1D ($d=1$) case, it is well known [?] that D can display an abrupt percolation-like transition from diffusive ($D > 0$) to sub-diffusive ($D = 0$) behavior, as the sparsity parameter drops below the critical value $s_c = 1$. Similar anomalies are found for fractal structures with $d < 2$, see [? ?]. A question arises whether such a transition might happen in higher dimensions. In [?] the spectral properties in the 2D ($d=2$) case have been investigated: on the basis of the renormalization group (RG) procedure it has been deduced that $\mathcal{P}(t)$ decays in a logarithmic way, indicating anomalous (sub) diffusion.

3.6 Variable range hopping

It should be clear that there are two major routes in developing a theory for D . Instead of deducing it from spectral properties as in [?], one can try to find ways to evaluate it directly via a resistor network calculation [? ? ? ? ?], leading in the standard Mott problem to the Variable Range Hopping (VRH) estimate for D . In [? ? ?] this approach has been extended to handle “sparse” banded matrices whose elements have log-wide distribution, leading to a generalized VRH estimate. In what follows we pursue the same direction and obtain an improved estimate for D that we call Effective Range Hopping (ERH). Using this approach we show that in the 2D case, as s becomes small, the functional $D[\mathbf{w}]$ exhibits a smooth crossover from “linear” behavior to “semi-linear” VRH-type dependence.

3.7 Sparsity vs percolation

The problem that we consider is a variant of the percolation problem [? ?]: Instead of considering a bi-modal distribution (“zeros” and “ones”) we consider a log-wide distribution

of rates [1], for which the median is much smaller than the mean value. We call such network “sparse” (with quotation marks) because the large elements constitute a minority.

3.8 Anderson localization

Disregarding the “sparsity” issue, the model that we are considering is a close relative of the Anderson localization problem. In the problem that we discuss here all the off diagonal elements are positive, while the negative diagonal elements compensate them. Since all the off diagonal elements are positive numbers, it is clear that we cannot have “destructive interference”, and therefore we do not have genuine Anderson localization. Therefore in general we might have diffusion, even in 1D. In 2D we have a percolation threshold, which is again not like Anderson localization. For further discussion see for example the discussion of fractons in [2].

3.9 Debye law

In the standard Anderson model the eigenvalues form a band $\lambda \in [-\lambda_c, \lambda_c]$. The states at the edge of the band are always localized. The states in the middle of the band might be de-localized if $d > 2$. The localization in a disordered elastic medium had been studied [?]. Disregarding the “sparsity”, it is the same problem that we are considering here. It has been found that the spectrum is $\lambda \in [0, \lambda_c]$. The ground state is always the $\lambda = 0$ uniform state. The localization length diverges in the limit $\lambda \rightarrow 0$. Consequently the Debye density of states is not violated: the spectrum is asymptotically the same as that of a diffusive (non-disordered) lattice. It follows that the survival probability should be like that of diffusive system, and therefore we also expect diffusive behavior for the transport: spreading that obeys a diffusion equation.

3.10 Analogy to an electrical circuit

We may think of a “ladder” of capacitors and resistors as portrayed in the diagram.

3.11 Analogy to a masses and springs mesh

The same network may describe equal masses (which we can simply define as 1) distributed in space, connected by springs. The locations of the masses will obey a second degree differential equation:

correct this! Where k_{nm} is the spring

3.12 msc

There are diverse examples for extended systems whose dynamics is described by a rate equation. This include in particular the analysis of "random walk" where the transitions are between sites of a network. Another example is the study of energy absorption due to Fermi-Golden-Rule transitions between energy levels. In both cases there are two common questions that arise: (1) What is the survival probability of a particle that has been prepared in a given site; (2) Is there normal diffusion or maybe only sub-diffusion, and how it is related to the survival probability.

In recent years there is a growing interest in systems where the transition rates have log-wide distribution. This means that the values of the rates are distributed over many decades as in the case of log-normal or log-box distributions. Such "glassy" or "sparse" systems can be regarded as a "resistor network", and the analysis might be inspired by percolation theory, variable range hopping phenomenology, and the renormalization-group methods.

While the theory of 1D networks with near-neighbour transitions is quite complete, the more general case of quasi-1D / 2D and possibly higher dimensions lacks a unifying framework, and there are numerous open questions that we would like to study as outlined below.

Modeling .– N interconnected sites constitute a network. A single particle is bound to the network. We denote by $p_n(t)$ the probability to find the particle on site n at time t , so that $\sum_n p_n(t) = 1$. The dynamics of the system are described by the rate equation:

$$\frac{dp_n(t)}{dt} = \sum_m W_{nm} p_m(t) \quad (3.3)$$

Where W_{nm} is the *transition rate*, i.e. the rate at which probability moves from site m to site n . Because of probability conservation, we want to have $\sum_m W_{nm} = 0 \quad \forall n$, which we can achieve by setting $W_{nn} = -\sum_{m \neq n} W_{nm}$, meaning that for each site the sum of incoming

transition rates negates the outgoing transitions. The rate equation can also be written as a vectorial equation: $\dot{\mathbf{p}} = \mathbf{W}\mathbf{p}$. In its basic form, the matrix \mathbf{W} is symmetric (at the moment, see "Assymetric VRH" further down in this section), except for the main diagonal, which has values that ensure that each row's sum is zero.

The network (the values of W_{nm}) can be defined arbitrarily, but we wish to focus on networks that represent geometric systems, by defining the transition rates to depend on the distance between randomly scattered points[?]. One such network, with the rates defined as:

$$W_{nm} = w_0 e^{(r_0 - r_{nm})/\xi} \quad (3.4)$$

Where r_{nm} is the distance between site n and m , r_0 is the typical distance between points, w_0 is the transition rate between points at distance r_0 , and ξ is a scaling coefficient. In general, we are going to define $r_0 = n^{-1/d}$, where $n = \frac{N}{V}$ is the site denisty, and we are going to rescale time by setting $w_0 = 1$. This model was studied in [?], and is of particular interest for us.

Dimensions.— The system may be in $1d$, $2d$, $3d$ etc., or in quasi- $1d$. The $1d$ system has been studied, among others, in[?][?][?]. Quasi- $1d$ relates either to $1d$ systems where there are bonds between sites beyond the nearest neighbors, or to $2d$ systems with finite width (strip). Both these systems have banded matrices, with bandwidth b .

Survival probability - $\mathcal{P}(t)$.— The survival probability is the probability to remain in the starting site. If the initial condition was $p_0(0) = 1$, $p_i(0) = 0$ for $i \neq 0$, then $\mathcal{P}(t) = p_0(t)$. The survival probability is directly related to the spectral properties of the transition matrices, and it can be shown that

$$\mathcal{P}(t) = \frac{1}{N} \sum_{\lambda} e^{\lambda t} \rightarrow \frac{1}{N} \int e^{\lambda t} g(\lambda) d\lambda \quad (3.5)$$

where the λ s are the eigenvalues of the matrix, namely that the survival probability is the Laplace transform of the eigenvalue density.

Transport and Spreading.— A particle can be transmitted through the system from one end to the other. This transport can be characterized in different ways. One way is to calculate the spreading $S(t)$, which is the variance (second moment) of the particle location, i.e:

$$S(t) = \sum_n (r_n(t))^2 p_n \quad (3.6)$$

Where r_n is the location of the n th site. The survival probability is related to the diffusion because of scaling considerations by:

$$\mathcal{P}(t) = \left(2\pi \frac{S(t)}{r_0^2}\right)^{-d/2} \quad (3.7)$$

By definition, diffusive systems obey:

$$S(t) = 2Dt \quad (3.8)$$

$$\mathcal{P}(t) = \left(2\pi \frac{S(t)}{r_0^2}\right)^{-d/2} = \left(4\pi \frac{Dt}{r_0^2}\right)^{-d/2} \quad (3.9)$$

We can combine this result with 3.5 to obtain a relation between $g(\lambda)$ and D :

$$g(\lambda) = \mathcal{L}^{-1}[\mathcal{P}(t)] = \mathcal{L}^{-1}\left[\left(4\pi \frac{Dt}{r_0^2}\right)^{-d/2}\right] = \frac{\lambda^{\frac{d}{2}-1}}{\Gamma\left(\frac{d}{2}\right) \left(4\pi \frac{D}{r_0^2}\right)^{d/2}} \quad (3.10)$$

$$C(\lambda) = \int_{\infty}^{\lambda} g(\lambda') d\lambda' = \frac{\lambda^{\frac{d}{2}}}{\frac{d}{2} \Gamma\left(\frac{d}{2}\right) \left(4\pi \frac{D}{r_0^2}\right)^{d/2}} \quad (3.11)$$

3.13 Spreading of wavepackets in the quantum case

3.14 Localization

Part II

Completed Work

Chapter 4

Completed Work

4.1 The ERH procedure

The diffusion coefficient is defined by the dependence of the variance in time:

$$\text{Var}(n) = 2d D t \quad (4.1)$$

Within the transient diffusion stage, assuming we start at a specific node n , the variance after time t will be

$$\text{Var}(n) = \sum_m w_{nm} t (x_m - x_n)^2 \quad (4.2)$$

Therefore, the diffusion coefficient for evolution starting at node n is

$$D_n = \frac{1}{2d} \sum_m (x_m - x_n)^2 w_{nm} \quad (4.3)$$

Averaging over the starting node, and converting the sum to an integral, we have

$$D_{\text{linear}} = \frac{1}{2d} \iint w(r, \epsilon) r^2 \rho(r, \epsilon) d\epsilon dr \quad (4.4)$$

4.2 The $d = 1$ lattice model

4.2.1 Exact and Numerical results

4.2.2 ERH calculation

4.3 The $d = 2$ lattice model

4.3.1 Numerical results

4.3.2 ERH calculation

Part III

Preliminary Analysis

Chapter 5

Introduction

Part IV

Appendix

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Appendix A

Published Papers

Appendix B

Spacing Statistics in d -dimensions

Appendix C

Resistor Network Calculation