Physics on graphs

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Contents

Motivation and Aim

Networks appear in many contexts, whether concretely in information management and transportation or abstractly when modeling interconnections of systems.

In this talk I will focus on three physical concepts, which can be formulated and discussed within the context of networks.

Motivation and Aim

- Propagation of waves
- Brownian motion
- Dynamical quantum theory

The precise mathematical notion of a network
we will use is a that of a

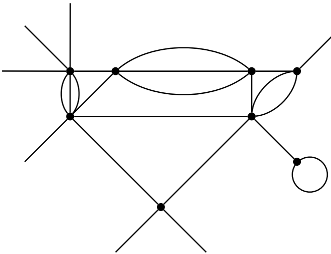
- Metric graph

With applications in mind this may be a highly idealized description. However, as we will see it will allow to use rigorous mathematical tools.

Metric graphs

Definition:

A metric graph $\mathcal{G}$ is a finite collection of half lines and finite intervals of given lengths with an identification of some of their endpoints (=vertices)



A graph with 8 vertices, 7 external and 17 internal edges and one tadpole.

Propagation of waves

Light can be described as a solution of equations carrying the name of James Clerk Maxwell (1831-1879). These equations were published in 1864. The experimental verification was done by Heinrich Hertz (1857 - 1894) in the year 1886. Special solutions for the electric and magnetic fields in the vacuum, that is in the absence of charges and currents, are of the form

$$\vec{E}(\vec{x}, t) = \vec{E}_0 \, \mathrm{e}^{\mathrm{i}(\omega t + \vec{k}\cdot\vec{x})}, \tag{1}$$
$$\vec{B}(\vec{x}, t) = \vec{B}_0 \, \mathrm{e}^{\mathrm{i}(\omega t + \vec{k}\cdot\vec{x})}.$$

The 3 vectors $\vec{E}_0$, $\vec{B}_0$ and $\vec{k}$ are pairwise orthogonal and $\vec{E}_0$ and $\vec{B}_0$ have equal length. Also $\vec{k}$ and ω are related by $\omega = \pm|\vec{k}|c$, where c is the speed of light.

Propagation of waves

As a consequence of being solutions of the Maxwell equations they also are solutions of the wave equation

$$\Box \vec{E}(\vec{x}, t) = 0, \qquad (2)$$
$$\Box \vec{B}(\vec{x}, t) = 0.$$

$\Box$ is the d'Alembert operator:

$$\Box = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta,$$

and Δ is the Laplace operator:

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}.$$

Propagation of waves

An important consequence is the property of

Finite propagation speed

Any (light) signal sent out at time $t = 0$ at the point $\vec{x}_0$ can arrive at the point $\vec{x}$ at time $t > 0$ only when the distance between $\vec{x}_0$ and $\vec{x}$ is exactly ct (and not earlier).

Propagation of waves

Instead of ordinary euclidean space $\mathbb{R}^3$ one may also consider a Riemannian manifold $\mathcal{M}$. In particular on $\mathcal{M}$ the notion of a distance between two points is well defined. On such a space there exists a canonical Laplace operator Δ, called the Laplace-Beltrami operator operating on functions on $\mathcal{M}$. So the d'Alembert operator is well defined. It operates on functions of $x \in \mathcal{M}$ and time t.

Again one can prove finite propagation speed.

Propagation of waves

Back to metric graphs:

They are singular spaces, the singularities being at the vertices. And this makes them interesting. Away from the vertices everything is fine: One can define the Laplace operator as the second derivative on functions on the graph away from the vertices. However, they have to satisfy boundary conditions at the vertices. Therefore there are many of them, according to the choice of such boundary conditions.

Brownian motion

However, one can find a nice class with the following property:

To any such Δ one can associate a d'Alembert operator $\Box$ such that the solutions of the associated wave equation satisfy the finite propagation speed property.

The boundary conditions specify the way in which a wave packet is split up when reaching a vertex.

Brownian motion

In 1829 Robert Brown published an article in the Philosophical Magazine, where he described " rapid oscillatory motion" of pollen in water. This phenomenon now carries his name: Brownian motion. He made many observations on different materials, organic and inorganic.

The first to provide a full fledged theory explaining this phenomenon were Albert Einstein (1905) and Marian Smoluchowski (1906), though there were precursors like Louis Bachelier (1900) in his thesis " The theory of speculation".

Brownian motion

Making some probabilistic assumptions Einstein derived the diffusion equation

$$\frac{\partial \rho}{\partial t}(\vec{x}, t) = D \Delta \rho(\vec{x}, t).$$

D is called the coefficient of diffusion. Thus if a Brownian particle starts (in three dimensional space) at time $t = 0$ at the point $\vec{y}$, that is $\rho(\vec{x}, t = 0) = \delta(\vec{x} - \vec{y})$, then

$$\rho(\vec{x}, t) = \frac{1}{(4\pi D t)^{3/2}} \mathrm{e}^{-\frac{|\vec{x} - \vec{y}|^2}{4Dt}}$$

gives the probability of finding the particle at x at time t. For the choice $D = 1$ the right hand side is called the heat kernel, that is the integral kernel of $\exp t\Delta$. Starting this, it is possible to construct what is now called a Wiener process, the mathematical description of a Brownian motion. For this reason, the Laplace operator is called the infinitesimal generator of the process.

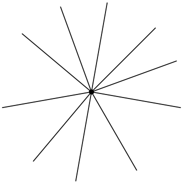
Brownian motion

Motivated by this we have found all self-adjoint Laplace operators Δ on any given graph, whose heat kernel $\exp t\Delta(p, q)$, with p and q being points on the graph, is positive. This is the essential ingredient, which allows one to construct a Wiener process on the graph.
However, there exist additional processes on any given graph, whose infinitesimal generators are non-selfadjoint Laplace operators. They satisfy different boundary conditions.

Brownian motion

They are given by local boundary conditions at each vertex

A single vertex grapoh is given by an arbitrary number $n = |\mathcal{E}|$ of half lines with one joint vertex



$\mathcal{E}$ = set of external half-lines e, each $\cong [0, \infty)$.

Brownian motion

At any such vertex v of the graph Wentzell's boundary conditions are of the form

$$af(v) - \sum_e b_e f'(v_e) + \frac{1}{2} c\, f''(v) = 0$$

with $a, b_e, c \geq 0$ and $a + \sum_e b_e + c = 1$.
f is a function on the graph, e labels an edge and $f'(v_e)$ denotes the outward derivative of f at v along the edge e. Also f is such its the second outward derivatives along each edge exist, are all equal. They are written as $f''(v)$.

Brownian motion

Interpretation of the parameters in these boundary conditions:

- $\beta = a/(1-a-c)$ describes the probability on an exponential scale that the Brownian particle will die, that is move to a cemetary, when it arrives at the vertex v.
- $\gamma = c/(1-a-c)$ measures a certain stickiness of the vertex, given by a slow down of the Brownian motion near the vertex.
- $$0 \leq w_e = \frac{1}{1-a-c} b_e,$$

  is the probability, that the Brownian particle, upon arrival at the vertex and unless it has died, will move from v continuously into the edge e.

Brownian motion

- Given such boundary conditions at each vertex gives a so called Feller process.
- Conversely the infinitesimal generator of each Feller process on the graph is a Laplace operator with boundary conditions of this form.

Open problem (not yet done) :

Study of processes, where the Brownian particle can jump from a vertex into an edge.

Quantum mechanics

In the year 1925 Erwin Schrödinger (1987 -1961) wrote down the equation

$$i\hbar\frac{\partial}{\partial t}\psi(t) = H\psi(t),$$

which carries his name. It is the time evolution equation for a quantum mechanical state $\psi(t)$. $\hbar$ $\psi(t)$ is an element of a complex Hilbert space and H is the Hamilton operator, a self-adjoint linear operator acting in this space.

This is a very general feature:

A dynamical quantum system is given by the specification of the Hilbert space and of H.

Quantum mechanics

An important example is the Hilbert space $L^2(\mathbb{R}^3)$ of all square integrable functions $\psi(\vec{x})$ on $\mathbb{R}^3$ and

$$H = -\frac{\hbar^2}{2m}\Delta + V(\vec{x}).$$

It provides the quantum mechanical description of a particle of mass m moving under the influence of a potential $V(\vec{x})$. For vanishing potential, one speaks of free motion.
Letting V be the Coulomb potential, Schrödinger was able to solve (with the help of Hermann Weyl) the stationary Schrödinger equation

$$H\psi = E\psi$$

for all energy eigenvalues of the hydrogen atom.

Quantum mechanics on graphs

Model on the graph $\mathcal{G}$:

The Hilbert space is $L^2(\mathcal{G})$, the set of all square integrable functions on $\mathcal{G}$ (= wave packets on $\mathcal{G}$) and the Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\Delta$$

where Δ is any self-adjoint Laplace operator. So this describes free motion of the quantum particle away from the vertices.

Local Kirchhoff law

Consequence of self-adjointness:

For a given state $\psi(x)$ define the quantum current

$$j(x) = \frac{\mathrm{i}}{2m}\left(\overline{\psi(x)}\frac{d}{dx}\psi(x) - \left(\frac{d}{dx}\overline{\psi(x)}\right)\psi(x)\right)$$

Then at any vertex v the following quantum version of the local Kirchhoff law holds:

$$\sum_{e: v\in\partial(e)} j(v_e) = 0,$$

that is the sum of the currents at each "node" vanishes.
So again the boundary conditions specify, how a wave-packet is split up, when it reaches a vertex.

Scattering theory

One may discuss scattering theory: Imagine a wave-packet under the time evolution entering the graph through one of its external edges.

Question: What happens asymptotically for large times?
The answer is given in form of the so called on-shell S-matrix at energy E, in this case it is a matrix

$$S(E)_{e\,e'},$$

where e and e' label the external edges of the graph $\mathcal{G}$. Using linear algebra, it can be calculated explicitly in terms of the boundary conditions, which define the Laplacian.

Kirchhoff's rule for quantum wires

This matrix is unitary:

$$\sum_{e} \overline{S(E)_{ee'}} S(E)_{ee''} = \delta_{e'e''}.$$

In particular when $e' = e''$: The probability for a quantum particle of energy E entering the graph at any external edge e' and leaving through any edge e equals 1.
In analogy to Kirchhoff's law for currents in electrical circuits, we coined the name

Kirchhoff's rule for quantum wires

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