

The heat equation and Brownian motion

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Introduction. This brief note is a supplement to the the more detailed material in [XX] which appears as a chapter in the extensive notes on analytic function theory from by course held at the department of mathematics in Abbis Abeba in February-March 2009. The heat equation has a long history whose physical relevance has inspired mathematicians to develop methods to obtain solutions. A major step was introduced by Fourier around 1810 which gives a recipe to solve the heat equation with prescribed boundary values. We restrict the discussion to the 2-dimensional case where the basic PDE-equation is

$$(*) \quad \frac{\partial u}{\partial t}(t, z) = \Delta(u)(z, t)$$

Here t is a time variable and $z = x + iy$ moves in a domain Ω of the complex plane. The PDE-equation corresponds to a Brownian motion in Ω . Suppose that the density of particles observed at time $r = 0$ is observed and expressed by a density function $g_0(z)$, i.e. g is real-valued and non-negative and its area integral over Ω is one. When $t > 0$ the classical laws in physics mean that the observed density at some time $t > 0$ is expressed by a density function $x \mapsto u(z, t)$ where u solves $(*)$ and satisfies the following boundary condition for every $t > 0$:

$$(1) \quad \frac{\partial u}{\partial n}(z, t) = 0 \quad : \quad z \in \partial\Omega$$

In addition one has an initial density distribution at time zero, i.e. $u(0, z) = g_0(z)$.

Schrödinger's boundary value problem. Quantum mechanics led to problems which from a mathematical point of view gives rise to non-linear equations of considerable interest for mathematicians. A precise question was raised by Schrödinger in his famous article *Théorie relativiste de l'électron et l'interprétation de la mécanique quantique* from 1932. The solution $u(x, t)$ above is not valid in the non-classical case while another density $z \mapsto f_1(z) \neq u(t_1, z)$ is observed at some time $t_1 > 0$. Thus, something highly improbable but nevertheless possible has occurred during the time interval $[0, t_1]$. Schrödinger asked for the most likely density a time t_1 . He concluded that that the requested time-dependent density $w(t, z)$ which substitutes $u(t, z)$ above, is found in a non-linear class of functions \mathcal{W} formed by products

$$u_0(t, z) \cdot u_1(z, t)$$

where $u_0(z, t)$ is a solution to the heat equation $(*)$ while u_1 solves the adjoint equation

$$\frac{\partial u_1}{\partial n}(z, t) = -\Delta(u_1)(t, z) \quad \text{for time values } t < t_1$$

and satisfies the boundary condition (1). Now one seeks a function $w(t, z)$ in the family \mathcal{W} which satisfies two boundary value conditions

$$(**) \quad w(0, z) = f_0(z) \quad : \quad w(t_1, z) = f_1(z)$$

where f_0, f_1 is a pair of *prescribed* density functions. The mathematical problem is now to determine a pair of functions $g_0(x) = u_0(x, 0)$ and $g_1(x, t_1) = u_1(x, t_1)$ such that $(**)$ holds. The solution to this problem can be transformed into a system

of non-linear integral equations. Namely, for the given domain Ω there exists the Poisson-Greens function $K(t, z, \zeta)$ and we have

$$\begin{aligned} u_0(t, z) &= \iint_{\Omega} K(t, z, \zeta) \cdot g_0(\zeta) d\xi d\eta \\ u_1(t, z) &= \iint_{\Omega} K(t_1 - t, z, \zeta) \cdot g_1(\zeta) d\xi d\eta \end{aligned}$$

Next, the boundary conditions for w yield

$$\begin{aligned} f_0(z) &= g_0(z) \cdot \iint_{\Omega} K(-t_1, z, \zeta) \cdot g_1(\zeta) \cdot d\xi d\eta \\ f_1(z) &= g_1(z) \cdot \iint_{\Omega} K(-t_1, z, \zeta) \cdot g_1(\zeta) \cdot d\xi d\eta \end{aligned}$$

Remark. Notice that the last two equations means that the requested pair of g -functions for a given pair of f -functions means that one has a non-linear system of integral equations. The solvability of this system was left open by Schrödinger but was put forward to the mathematical community at the IMU-congress in Zürich 1932 in the plenary talk by Serge Bernstein. In 1940 Fortet published the article *Résolution d'un système d'équations de Schrödinger* which gave a methods for approximating solutions under some specific conditions on the boundary data. A general method to find solutions to a non-linear system as above was introduced by Beurling in the article [Beurling]. It is exposed in § XX from Special sections and demonstrates the existence of solutions to the system above for smooth domains in \mathbf{R}^2 . Beurling's theoretical solution is implicit since it is established via a certain non-linear variational problem for product measures defined via Poisson-Green's function.

The classical heat-equation. From now on we restrict the study to the ordinary heat equation. We shall not attempt to expose all details about this equation since it would require an extensive chapter in PDE-theory. Let us only remark that (*) is an example of a parabolic equation for which uniqueness and existence of solutions with prescribed initial conditions were studied at an early stage by Gevrey, Hadamard and Holmgren. More recent progress was achieved by Petrowsky, Khintchine and Kolmogorov which established the relation between solutions to heat equations and stochastic processes.

An notable point is that the heat equation can be rewritten as an integral equation. This was already used in pioneering work by Ivar Fredholm and leads to existence theorems and insight about associated eigenvalues and eigenfunctions under quite general boundary value conditions. We shall restrict the discussion to the heat equation in the complex domain where results about Green-kernels from Chapter V can be applied. Let $z = x + iy$ be a complex variable and Ω is a domain whose boundary consists of p many closed and disjoint differentiable Jordan curves. Here p is some positive integer and the case $p = 1$ is not excluded. In Chapter V we constructed the Green's function $G(z, \zeta)$ defined in the closed product $\bar{\Omega} \times \bar{\Omega}$. Denote by $C_*(\Omega)$ the Banach space of continuous functions in $\bar{\Omega}$ which are zero on the boundary. Then there exists the linear operator from this Banach space into itself defined by

$$Tu(z) = \iint_{\Omega} G(z, \zeta) u(\zeta) \cdot d\xi d\eta$$

Recall from §§ in Chapter V that if ϕ is a C^2 -function with compact support in Ω then

$$\iint_{\Omega} \Delta(\phi)(z) \cdot u(\zeta) dx dy = \iint_{\Omega} \phi(z) \cdot Tu(\zeta) dx dy$$

This equation means that Tu regarded as a distribution has a Laplacian expressed by the continuous density u , i.e. one has the equality

$$\Delta(Tu)(z) = u(z) \quad : \quad z \in \Omega$$

Let $u \in C_*^0(\Omega)$ be an eigenfunction where

$$u(z) = \mu \cdot Tu(z)$$

holds for some non-zero constant μ which by the above gives

$$\Delta(u) = \frac{1}{\mu} \cdot u$$

In particular u is of class C^2 in Ω and Green's formula gives:

$$\mu \cdot \iint_{\Omega} \Delta(u)(z) \cdot u(z) dx dy = \iint_{\Omega} \nabla(u)^2(z) \cdot dx dy = 0$$

where $\nabla(u)^2 = u_x^2 + u_y^2$. Hence the eigenvalue μ is real and strictly negative.

1. The spectrum of T and the function $\mathcal{D}(\lambda)$. Set $G^{(0)} = G$ and define inductively

$$G^{(m)}(z, \zeta) = \mu \cdot \iint_{\Omega} G(z, \zeta) \cdot G^{(m-1)}(z, \zeta) \cdot d\xi d\eta$$

Let λ be a new complex parameter and put

$$\mathcal{D}(\lambda) = \sum_{m=0}^{\infty} \lambda^m \cdot G^{(m)}(z, \zeta)$$

We regard $\mathcal{D}(\lambda)$ as a function with values in the Hilbert space of square integrable functions on the product $\Omega \times \Omega$, i.e. we use that

$$\iint_{\Omega \times \Omega} |G(z, \zeta)|^2 \cdot d\xi d\eta dx dy < \infty$$

and similar finite double integrals occur for the functions $\{G^{(m)}\}$. With these notions one has the general result below which was established by Carleman in already in 1918 based upon previous inequalities due to Fredholm, Hadamard and Hilbert.

2. Theorem. *The function $\mathcal{D}(\lambda)$ extends to a meromorphic function in the whole complex λ -plane whose poles are confined to a sequence of strictly negative real numbers.*

3. The heat equation. Let $\{\lambda_k\}$ be the poles of \mathcal{D} . If the pole has multiplicity $e_k \geq 2$ the corresponding eigenspace is e_k -dimensional. Repeating eigenvalues with eventual multiplicities we obtain a sequence of eigenfunctions $\{u_k\}$ with eigenvalues $\{\lambda_k\}$ and for each k the eigenfunction u_k is normalised so that

$$\iint u_k^2(x, y) \cdot dx dy = 1$$

and chosen so that they form an orthonormal set in the Hilbert space $L^2(\Omega)$. Notice that every u -function is real-valued. Next, let t be a new real parameter which serves as a time variable. If $\{c_k\}$ is a sequence of complex numbers we set

$$p(t, z) = \sum_{k=1}^{\infty} c_k \cdot e^{-\lambda_k t} \cdot u_k(z)$$

The series converges nicely when $t > 0$ if $\{c_k\}$ do not increase too rapidly and the p -function satisfies the PDE-equation

$$\frac{\partial p}{\partial t} = \Delta(p)$$

when $t > 0$ and $z \in \Omega$. Next, the sequence $\{c_k\}$ determines an initial condition which usually is interpreted via a limit

$$\lim_{t \rightarrow 0} p(t, z) = p_*(z)$$

where $p_*(z)$ is a distribution. If p_* belongs to L^2 we have for example

$$c_k = \iint p_*(z) u_k(z) \cdot dx dy$$

4. The Brownian motion. As explained in §§ solutions to the heat equation correspond to probability densities for a particle whose time-dependent change of position is governed by a Brownian motion. For example, if $z \in \Omega$ is given and the particle starts at z at time zero then we consider the probability distribution:

$$t \mapsto \text{Prob}(z, t)$$

which gives the probability that the particle stays in Ω up to time t . Since Ω is bounded the particle eventually hits the boundary where it is absorbed. It means that

$$\lim_{t \rightarrow \infty} \text{Prob}(z, t) = 0$$

On the other hand the particle stays in Ω with high probability under short time intervals, i.e.

$$(1) \quad \lim_{t \rightarrow 0} \text{Prob}(z, t) = 1$$

Above (i-ii) hold for every $z \in \Omega$. The function

$$p(t, z) = \text{Prob}(z, t)$$

satisfies the heat equation and by (1) given by the series

$$(*) \quad p(t, z) = \sum c_k \cdot e^{-\lambda_k t} \cdot u_k(z) \quad \text{where} \quad c_k = \iint_{\Omega} u_k(z) \cdot dx dy$$

4.1 The E -function. When the particle starts at a point z the expected time before it hits the boundary is given by the equation:

$$E(z) = - \int_0^\infty t \cdot \frac{\partial p}{\partial t}(t, z) \cdot dt$$

Since p satisfies the heat equation and the differential operators ∂_t and the Laplacian of the independent z -variable commute with, it follows that

$$\Delta(E)(z) = - \int_0^\infty t \cdot \frac{\partial^2 p}{\partial t^2}(t, z) \cdot dt$$

After a partial integration we find that

$$\Delta(E)(z) = -1$$

Hence the function

$$E(z) + \frac{|z|^2}{2}$$

is harmonic in Ω and since $E = 0$ on the boundary we conclude that

$$E(z) = \int_{\partial\Omega} P_z(\zeta) \cdot \frac{|\zeta|^2}{2} \cdot d\xi d\eta - \frac{|z|^2}{2}$$

where $P_z(\zeta)$ is the Poisson kernel which exhibits solutions to the Dirichlet problem.

4.2 Example. Let $\Omega = \{|z| < R\}$ be a disc. Then

$$E(z) = \frac{1}{2}(R^2 - |z|^2)$$

Next, let $\Omega = \{1 < |z| < R\}$ be an annulus. Then the reader may verify that

$$E(z) = \frac{R^2 - 1}{2} \cdot \frac{\log |z|}{\log R} + \frac{1 - |z|^2}{2}$$

Notice that E takes its maximum over the circle of radius r^* where

$$r^* = \sqrt{\frac{R^2 - 1}{2 \log R}}$$

The reader is invited to interpretate the formulas above by probabilistic considerations.

4.3 Points of arrival. Let ω be some finite union of open subintervals of $\partial\Omega$. Starting the Brownian motion at a point $z \in \Omega$ we can consider the paths which at the first arrival to the boundary hits points in ω . Again we get a p -function which satisfies the heat equation but here the initial condition is different and depends upon ω . More precisely, the probability that a Brownian path escapes for the first time at a point in ω is given by the value of the harmonic measure function $\mathbf{m}(\omega, z)$. Now we define the function

$$p_\omega(t, z) = \sum c_k(\omega) \cdot e^{-\lambda_k \cdot t} \cdot u_k(z)$$

where $\{c_k(\omega)\}$ are determined by

$$c_k(\omega) = \iint_{\Omega} \mathbf{m}(\omega, z) \cdot u_k(z) \cdot dx dy$$

4.4 A joint probability distribution. Let ω be some open set of $\partial\Omega$ as above and $t > 0$ some fixed time-value. With a small δt we seek the probability that the particle which starts at some z , escapes at some point in ω for the first time during the interval $[t, t + \delta t]$. From the above this probability up to small order of δt is given by:

$$\left[\sum c_k(\omega) \cdot \lambda_k \cdot e^{-\lambda_k \cdot t} \cdot u_k(z) \right] \cdot \delta t$$

4.5 Example. Suppose that the "open window" which the particle wants to hit on the boundary changes with time. The probability that it will escape through the changing window becomes

$$(*) \quad \sum \left[\int_0^\infty c_k(\omega_t) e^{-\lambda_k t} \cdot dt \right] \cdot \lambda_k \cdot u_k(z)$$

4.6 A special case. Suppose that Ω is the unit disc and $z = 0$ the starting point. Let $0 < a < \pi$ and suppose that the interval ω_t is $(-a \cdot |\sin \gamma t|, a \cdot |\sin \gamma t|)$ where $\gamma > 0$ is a constant. So the window is closed when $t = 0$ and has maximal width at time values when $|\sin \gamma t| = 1$. Here we have:

$$c_k(\omega_t) = \frac{a \cdot |\sin(\gamma t)|}{\pi}$$

4.7 Remark. The reader may consult text-books for the classic formulas which determine the sequence of eigenvalues $\{\lambda_k\}$ and the sequence $\{u_k(0)\}$ in a disc.

So admitting this one has a formula for the probability to escape the changing window. However, a computer should be used to obtain a numerical value. Let us also remark that one can also employ Monte Carlo simulations to determine (*) above. More precisely one instructs the computer to change the size of the open window and efficient use of MathLab provide accurate approximations and there is no difficulty to extend the situation to the case when one starts from an arbitrary point in D . One can go further and replace the special "opening function" $|a| \cdot |\sin \gamma t|$ by other time dependent functions and numerical solutions are obtained via Monte Carlo simulations, i.e. we get approximative values for the probability to escape a moving window on the boundary of an arbitrary domain in $\mathcal{D}(C^1)$.

Passing to higher dimensions where the case $n = 3$ is of special interest one can still employ Monte Carlo simulations and establish numerical values for many different expected values as well as higher moments and other joint distributions.

4.8 More involved problems. Above we were content to express various distribution functions for the time of first arrival to the boundary. One can also ask for positions of a particle during the time interval before it hits the boundary. Consider the case when $\Omega = D$ is the unit disc and the Brownian motion starts at the origin. On the circle we consider some interval $\omega = \{e^{i\theta} - 1 \mid \theta < a\}$ for some $0 < a < \pi/2$. Now we pursue the family of Brownian paths which hit on their first arrival to T hit points in ω . It is intuitively clear that these paths are not symmetrically distributed, i.e. a majority has a drift towards points on the interval ω . The distribution function $p(t)$ for the time of arrival was determined before. But we can introduce many other probability densities. For example let D_r be the disc of radius $r < 1$ centered at the origin. Given the interval ω above we consider the sample space \mathcal{B}_ω of all Brownian paths which start at the origin and hit ω on their first arrival to the unit circle. Every $\gamma \in \mathcal{B}_\omega$ visits the open disc D_r during some union of time intervals $\{t_k, T_{k+1}\}$ and let $\tau(\gamma) = \sum (t_{k+1} - t_k)$ be the total time while γ is in D_r until it eventually escapes and hits ω . So here

$$\gamma \mapsto \tau(\gamma)$$

is a random variable and one may ask for its expected value and also for higher moments and even its probability distribution will depend upon the pair a and r . It appears that problems of this kind have not been fully studied in analysis, i.e. one should first discover "closed analytic formulas" and after Monte Carlo simulations can be used to get numerical solutions. Notice that one can continue and pose many problems of this kind where various obstacles and changes of barriers occur. Thus, in principle there is an unlimited number of questions. But of course one should try to find questions with relevance to some natural model in science. However, from a mathematical point of view the search for analytic solutions to problems described above appears to be promising. Of course, exactly as in the case of the heat equation such solutions are still implicit since they for example may require that an infinite family of eigenvalues and associated eigenfunctions have been found via some PDE-equation. But here a pure theoretical problem is to set up such equations.

Stochastic optimization. Consider a random motion, which for simplicity is taken as the standard additive Brownian motion or its geometric counterpart with a time-independent volatility. Now one can study optimization problems where one seeks to maximize the expected value of a function which is called a profit function and is denoted by Π . Classic examples were considered by Bachelier in his article *La Bourse* from 1900 and was later been adopted into "mathematics of finance" under the name of "american options". This leads to free boundary problems whose analytic solutions are not known. Here is an example of such an optimization

problem: Let $[0, T]$ be a fixed time interval. At time $t = 0$ the stock market price of a risky asset is known to be K_0 and when t increases the price changes according to a geometric Brownian motion with constant volatility σ and some deterministic rate of increase μ . The owner of this risky asset has paid in advance an insurance J which gives the right to sell the asset at time T for a fixed price K_* which does not depend upon the actual stock market price $K(T)$, i.e. even if $K(T) < K_*$ the owner will receive the amount K_* which we for example measure in US-dollar. If $K(T) > K_*$ the owner is obliged to sell the asset at the current prize. One may imagine a person who will need all accumulated capital at time T or that the asset in question is no longer open to share-holders at the terminal time T .

During the time interval the stock-market price $K(t)$ changes in a random way and the owner has the alternative to sell the asset at any time and receive $K(t)$ which after is kept in a bank with some rate of interest r which at time T gives the profit

$$e^{rT} - t \cdot K(t)$$

In this model one may imagine that $r > \mu$ and it is therefore be tempting to sell the asset at some time $t < T$ provided that $K(t)$ is relatively high. The optimisation problem is to find the critical curve $t \mapsto K^*(t)$ where the owner maximizes expected net profit by selling the asset at the time moment when $K(t)$ for the first time is equal to $K^*(t)$. So here the curve $t \mapsto K^*(t)$ constitutes the free boundary. The analytic solution is not known for this curve even when volatility, μ and r are constants. However, numerical solutions are available using Kolmogorov's backward equation, and for this specific example many implemented in computer programs calculate values of options in financial affairs, In more serious applications to real science similar free boundary value problems also occur. But they are often governed by more involved equations via physical laws and very difficult problems arise when one leaves the "standard parabolic systems" and enter general non-linear PDE-equations of the parabolic or the hyperbolic type. For such problems advanced numerical analysis is needed which goes far beyond the rather trivial use of Monte Carlo simulations, though one should admit that the numerical solutions which are achieved by Monte Carlo methods are both instructive and sometimes also useful in applications; though last year's disaster in the world-wide financial market system might have put severe doubt upon various models in economics. But for scientific situations which arise in engineering, physics and chemistry the use of Monte Carlo simulations is a valuable tool.