Reading & Tutorial 2 (M 5339)

Reading and practice questions on text §1.3-§1.6.

(1) (Derivation of heat equation) Denote by $u = u(t, x)$ the temperature. The amount of heat (in calories, say) contained in a region Ω is given by

$$H(t) = \iiint_\Omega a\rho u dx$$

where a is the specific heat of the material and ρ the density. The rate of change in heat is $H'(t) = \iiint_\Omega a\rho u_t dx$.

Fourier's law says that heat flows from hot to cold regions proportionately to the temperature gradient. The heat energy on Ω is conserved when transferring through the boundary.

$$\frac{d}{dt}H(t) = \iiint_{\partial\Omega} \kappa(\nabla u \cdot n)dS$$

here κ is the heat conductivity that is a proportionality factor. We obtain by divergence theorem

$$\iiint_\Omega \nabla \cdot \mathbf{F}dx = \int_\partial \mathbf{F} \cdot \mathbf{n}dS$$

(see [Strauss, 1.3,#9], or Appendix 3)

$$\iiint_\Omega a\rho u_t dx = \iiint_\Omega \kappa\,\mathrm{div}(\nabla u)dx$$
$$\Rightarrow a\rho u_t = \kappa\,\mathrm{div}(\nabla u) \qquad (\textit{heat equation})$$

since Ω is arbitrary in $\mathbb{R}^3$.

(2) (Derivation of a Transport equation, [Strauss 1.3]).

The theory of PDE arises in physics and the study of this subject has motivated the mathematical development in analysis (multidimensional calculus, variational calculus, Fourier analysis, potential theory, dynamical systems) and geometry, as well as mathematical physics. These were developed from the second half of the eighteenth century, until the 1930s, from D'Alembert, Euler, and Lagrange to Poincare, Hilbert and von Neumann. PDE finds its applications in from hydrodynamics, celestial mechanics, continuum mechanics, elasticity theory, acoustics, thermodynamics, electricity, magnetism, optics, aerodynamics to atomic and subatomic theory to string theory. Physicists who are among the well-known to have profound influence in the areas are Newton, Maxwell, Bohr, Einstein, Heisenberg, Schrödinger, Dirac, Schwarzschild, Feynman, Boltzmann et al.

Following [Strauss] we give a derivation of

$$u_t + cu_x = 0 \qquad (1)$$

as follows. Let us say, we have a water fluid flowing at a constant speed c along a pipe of constant shape cross section (in the x-direction). Denote $u = u(t, x)$ the concentration (grams per centimer) at time t for the substance (say a pollutant) in the water.

On any given interval $[a, b]$ the amount of pollutant is given by

$$\int_a^b u(t, x)dx = \int_{a+ch}^{b+ch} u(t + h, x)dx$$

where the second in the equation means or reflects the fact that at time $t + \Delta t = t + h$, the amount of molecules of the pollutant stay the same along the flow.

Now take derivative in b to get $u(t, b) = u(t + h, b + ch)$. Then take derivative in h to obtain (1)

‡This equation tells that the rate of change of the concentration is proportional to the gradient.

(3) (Vibrating string: Derivation of a wave equation). Consider a flexible elastic homogenous string or thread of length L, that undergoes small transverse vibrations. Denote by $u(t, x)$ the displacement from equilibrium at t and x. Assume the tension is directed in the tangential direction along the string (due perfect flexibility) and assume that $T = T(t, x)$, the magnitude of the tension, is constant due to the homogeneity. Consider any portion $[a, x]$ of density ρ. By Newton's law, we have two equations in the longitudinal and the transverse components

$$\begin{aligned} T\frac{1}{\sqrt{1+u_x^2}}\Big|_a^x &= 0 \\ T\frac{u_x}{\sqrt{1+u_x^2}}\Big|_a^x &= \int_a^x \rho u_{tt} dx \end{aligned}$$

here the left hand side means the difference of the tension at a and x respectively at time t.

We neglect the small terms u and u_x to obtain

$$Tu_x(t, x) - Tu_x(t, a) = \int_a^x \rho u_{tt} dx$$

Take derivative in x to obtain (2)

$$\begin{aligned} Tu_{xx} &= \rho u_{tt} \\ u_{tt} &= c^2 u_{xx} \end{aligned} \tag{2}$$

where $c = \sqrt{T/\rho}$ indicates the wave speed. There are variations/modificatons of the wave equation subject to transverse elastic force, air resistance or external force.

(4) Laplace equation $\Delta u = 0$ (u called harmonic functions) describes the sate of stationary waves and diffusions where physical state u does not change with time. e.g the temperature of the object eventually attains its equilibrium state.

(5) Hydrogen atom. Think that we have an electron moving around a proton. Let $\hbar$ denote the Planck's constant. Let m and e be the mass and charge of the electron. Then the motion of the particle is given by a *wave function* $u(t,x,y,z)$ satisfying the Schrödingier equation

$$i\hbar u_t = -\frac{\hbar^2}{2m}\Delta u + Vu \tag{3}$$

where $V = -Ze^2/r$ is the potential with Z the atomic number for the case where the atom has a single electron only (e.g. a helium ion). In the hydrogen atom $Z = 1$.

Schrödingier theory postulates that The wave function u stands for a state of the particle (electron) where if R is any region in the space, then the probability of finding the particle in R at time t is given by

$$\iiint_R |u|^2 dxdydz$$

so that physically $|u|^2$ means the probability density.

The structure of the whole chemistry (atoms and molecules) thus can be explained by (3). Schrödinger interpretation

$$u \mapsto \mathbf{x}u \quad \text{refers to the position vector}$$
$$u \mapsto -i\hbar\nabla u \quad \text{refers to the momentum vector}$$

so that

$$\langle zu \mid u\rangle = \iiint z|u|^2 dxdydz \quad \text{is expected z coordinate of the position of electron}$$

$$\langle -i\hbar u_z \mid u\rangle = \iiint -i\hbar u_z \bar{u} dxdydz \quad \text{is expected z coordinate of the momentum of electron}$$

(6) (N-body system) For N particles

$$i\hbar\frac{\partial u}{\partial t} = -\sum_{i=1}^{N}\frac{\hbar^2}{2m_i}\Delta_{\mathbf{x}_i} u + V(\mathbf{x}_1,\dots,\mathbf{x}_N)u \tag{4}$$

In [Struass] it says "Except for the hydrogen and helium atoms (the latter having two electrons), the mathematical analysis is impossible to carry out completely and cannot be calculated even with the help of the modern computer." However, using various approximations (including theoretical and numerical ones) "many of the facts about more complicated atoms and the chemical binding of molecules can be understood."

‡The update is that recent years there have been remarkable progress on certain solutions to the N-body system by people in analysis and PDE. (the result along with the method are not simple though).

Ex. [Strauss, 1.3, #1] Derive the equation of the string motion in a medium in which the resistance is proportional to the velocity.

Ex. [Strauss, 1.3, #6] Consider the heat flow in a long circular cylinder where the temperature depends only on t and on the distance $r = \sqrt{x^2 + y^2}$ to the axis of the cylinder. From the three-dimensional heat equation derive the equation $u_t = \kappa(u_{rr} + \frac{1}{r}u_r)$.

Ex. [Strauss, 1.3, #9] Homework exercise! (aug.25,14)

Ex. [1.3,#10] If $f(x)$ is continuous and $|f(x)| \le (1 + |x|^3)^{-1}$ for all x, then

$$\iiint \operatorname{div} f dx = 0$$

[hint: divergence theorem]

Ex. If $\operatorname{curl} \mathbf{u} = \mathbf{0}$ for all x in $\mathbb{R}^3$, then there exists a function ϕ so that

$$\mathbf{v} = \nabla\phi.$$

(Recall that in ODE or Calc III, such field u is conservative $\iff$ line integrals from A to B are path-independent!)

Ex. [Strauss 1.5] Well-posedness problems

A PDE in a domain together with a set of IC or BC (or other auxiliary conditions) is said to be well-posed if the following fundamental properties are satisfied

- **a.:** Existence
- **b.:** Uniqueness
- **c.:** Stability. The unique solution u depends in a stable manner on the data of the problem. Namely, if the data change slightly, then it requires that the corresponding solution changes slightly also. This is indeed a very big question since there are many ways to measure the "continuous dependence of u on certain data".

Ex. [Strauss 1.5, #1]

Ex. [Strauss 1.5, #3]

Ex. [Strauss 1.5, #5]

Ex. [Strauss 1.5, #6]

(7) (Section 1.6, Types of 2nd-order equations)

Ex. [Strauss 1.6, #1]

Ex. [Strauss 1.6, #2]

Ex. [Strauss 1.6, #6]

(8) (optional reading**) Numerical methods: (a) Finite difference

[**Chapters 8, 13, 14, $u_{xx} \approx \frac{u(x+h,y)-2u(x,y)+u(x-h,y)}{h^2}$]

(b) FEM solver of PDE in 2D and 3D