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Exam in TFY4235 Computational Physics

May 04, 2015
09:00

Allowed help: Alternativ A

This problem set consists of 11 pages.

This exam is published on Monday, May 4 at 09:00 hours. You can work on your solution till **Thr. May 07, 2015 at 23:00** (“the deadline”). Before the deadline you should submit your final report in pdf-format via the “its leaning” page of this class. You are prior to this deadline *also* expected¹, to email the final report to me at Ingve.Simonsen@ntnu.no with subject TFY4235.²

Should you run short on time, you are advised to spend the time to do properly what you do instead of following a strategy of doing a little bit here-and-there.

Information posted during the exam, like potential misprints, links to papers etc. will be posted on the web-page of the course at <http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/#Exam> and/or <http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Exam/>. *It is your responsibility to check this information regularly!*

There is no restriction on the aid you can use in connection with this exam, including discussing it with anybody. *But, the report and the programs you will have to write yourself. Please attach your programs as appendices to the report. Give as a footnote the names of your collaborators during the exam.* The report may be written in either Norwegian (either variation) or in English.

There are no formal requirements for the format of the report in addition to what was said above. The report should explain what you have been doing, your results, and how you interpret these results. Details should be included to the extent that we as graders can follow your way of reasoning. General background theory that, for instance, can be found in textbooks, is not needed in the report. It is documentation of your work we are interested in!

¹Useful in the unlikely event that something should go wrong with the its learning submission.

²Warning: If your email is too large, the gmail system, to which I also forward my email, may notify you that the message was too large to be delivered to my gmail account. This means that your message was received successfully by the ntnu email system, if you were not informed otherwise.

Remember that if you have written an original and clever code for solving the problem, but are not able to explain it well in the report, it is hard to give you full credit.

I plan to have office hours from 13:00-16:00 on Monday May 04 in case you have questions to the problems. Only the two first days of the exam will I be present at the department.

Good luck to all of you!

Problem 1

Your suggested solution for *Assignment no 2* [1] should be handed in as part of the report. It will count 15% towards the final grade of the course.

Problem 2

Below we present the problems to be addressed in this takehome exam. In the following subsection, an introduction to the problem is given, while the actual tasks that you are asked to solve, are presented thereafter. Finally, in the appendix we have given some more technical background that may, or may not, be useful to you.

Introduction

From experience you know that a large drum (or tambourine) typically makes a lower tone than a small drum. Hence, from the tone that a drum makes, you can potentially say something about its size (area of the membrane).

What now if the area of the drum is the same, but we change the shape of the drum? Will this change of shape modify the tone of the drum? In 1966, the Polish mathematician Mark Kac, published a seminal and influential paper related to this question under the title “Can one hear the shape of a drum?” [2]. Several alternative ways of formulating this question do exist: Can the shape of the drum be predicted if its eigenfrequencies are known? Are the eigenfrequencies of a drum fingerprints of its shape? When publishing his paper [2], M. Kac did not know the answer to these questions. It should be pointed out that Kac was not the first to consider these issues; for instance, decades earlier (in 1911), Hermann Weyl did address this and related questions.

The question posed by Kac remained open for almost 30 years; today its answer (in two-dimensions) is: for many shapes, one cannot hear the shape of the drum completely, but some information can be inferred. For instance, the surface area of a drum, A , can be inferred from the expression

$$A = 4\pi \lim_{\omega \rightarrow \infty} \frac{N(\omega)}{\omega^2}, \quad (1)$$

where $N(\omega)$ denotes the number of eigenfrequencies (including degeneracy) smaller than ω . The function, $N(\omega)$, is known as the *integrated density of states* (IDOS). Furthermore, Hermann Weyl conjectured that the next term in the asymptotic of $N(\omega)$ would give the perimeter of the drum, i.e. in the limit of large ω one should have

$$N(\omega) = \frac{A}{4\pi} \omega^2 - \frac{L}{4\pi} \omega + \dots, \quad (2)$$

where L is the length of the perimeter of the drum and the dots mean lower order terms. Equation (2) is today known as the *Weyl-conjecture* for the IDOS, and under the assumption of a smooth boundary, it was proven to be correct in 1980. For additional details the interested reader is referred to, e.g., Refs. [3, 5, 6].

If the boundary of the drum is *fractal*, and therefore not smooth, what will then happen? A drum which has a fractal perimeter we will refer to as a *fractal drum*. In the early 1990s,

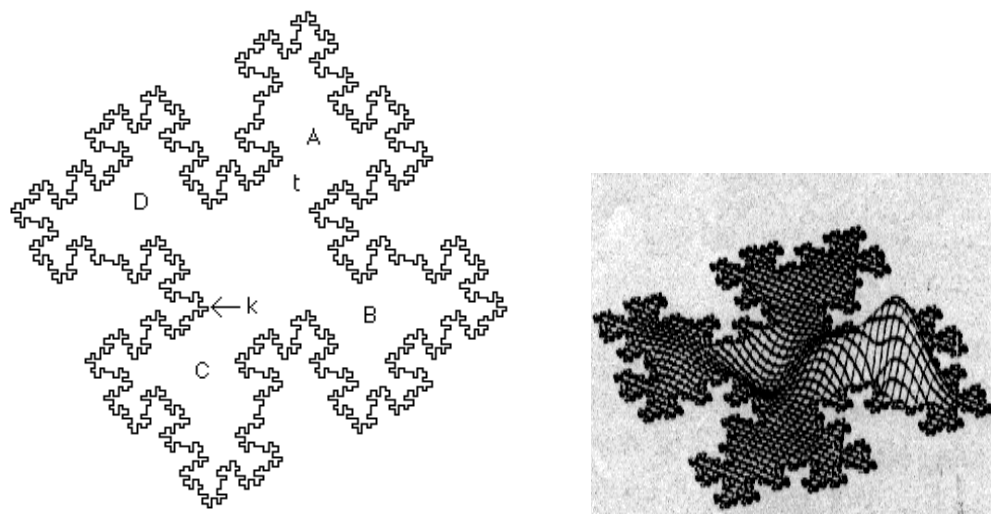


Figure 1: The boundary of the (quadratic Koch curve) fractal drum studied by Sapoval et al. [4]. Only the 3rd generation of the fractal is shown. The limiting curve for the shape has fractal (box-counting) dimension $\ln(8)/\ln(4) = 3/2$.

Sapoval and coworkers [4] conducted a series of elegant experiments to study the modes of fractal drums. A membrane stretched across a fractal perimeter [Fig. 1] was excited acoustically and the resulting modes observed by sprinkling powder on the membrane and shining laser light transverse to the surface. Sapoval observed modes *localized* to bounded regions, labeled *A*, *B*, *C*, and *D* in Fig. 1. In fact, by carefully displacing the acoustic source, Sapoval was able to excite each separately. Familiar (or “normal”) drums do not behave this way. Striking any part makes the whole membrane vibrate. Why is the fractal drum so different?

Sapoval showed that the equation governing wave motion has solutions with very large amplitude at the inward-facing corners, such as the point *k* in Fig. 1. These large amplitude regions generate a cascade of large amplitude vibrations that interfere with one another. This gives rise to dissipation on many scales, so fractal drums exhibit very strong damping. How does this explain the local vibrations of the fractal drum? The narrow throat *t* slows a wave traveling from *A* to *B*, and the strong damping absorbs the wave before it can spread. A simulation of one of these local modes is shown to the right in Fig. 1 (see also Ref. [4]). We remind you that any such local mode can be considered a linear combination of the eigenmodes of the system; the numerical calculation of the possible eigenmodes of the fractal drum is one of the main purposes of this exam and we will return to this problem below.

So how will the scaling of eigenmodes be for the fractal drum? This question was addressed by Sir M. Berry in 1979, and resulted in the Weyl-Berry conjecture. In a slightly modified form, the Weyl-Berry conjecture reads [5, 6]

$$N(\omega) = \frac{A}{4\pi}\omega^2 - C_d M \omega^d + \dots \quad (3)$$

In Eq. (3), d denotes the dimension of the perimeter of the drum and C_d and M are constants. It should be noted that $d = 1$ for a smooth perimeter of a two-dimensional drum something which is consistent with the Weyl conjecture (2).

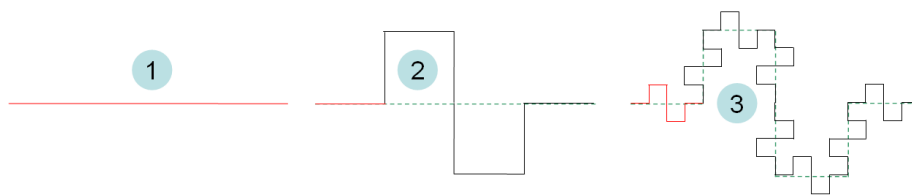


Figure 2: The process of constructing the fractal. (1) initial line segment (level $\ell = 0$); (2) “the generator” (level $\ell = 1$); (3) level $\ell = 2$ of the construction.

For the transition from a smooth square drum of area A to a fractal drum of the same area, the quantity of interest is

$$\Delta N(\omega) = \frac{A}{4\pi} \omega^2 - N(\omega). \quad (4)$$

According to the Weyl-Berry conjecture (3) this quality is expected to scale as $\Delta N(\omega) \sim \omega^d$, but what is the value of d for a given perimeter?

Exam questions

This exam is devoted to the numerical calculation of the eigenfrequencies and related eigenmodes of fractal drums and some related questions. As the perimeter of the fractal drum, we have chosen the so-called quadratic Koch curve (see Fig. 1), the same structure used in the experiments by Sapoval et al. [4].

Generation of the fractal: A quadratic Koch fractal is generated recursively by starting from a square of sides L . Next the generator labeled 2 in Fig. 2 is applied to each of its sides. This results in level $\ell = 1$ of the quadratic Koch fractal. To get to level $\ell = 2$, the generator is applied to each of the 32 line segment of the structure from the previous level ($\ell = 1$). By following this procedure level-by-level, one eventually arrives at the quadratic Koch fractal. The process applied to a horizontal segment is presented for level $\ell = 0$, $\ell = 1$ and $\ell = 2$ in Fig. 2. Moreover, the quadratic Koch fractal at level $\ell = 3$ is presented to the left of Fig. 1. Note that the generator, as shown at the center of Fig. 2, is obtained from a line segment of length s by dividing it into four equal pieces (each of length $s/4$); raising the 2nd element (from the left) a distance $s/4$ from the base; lowering the 3rd element a distance $s/4$, while the elements connected to the end points are not moved. It is customary to treat the central vertical part of the generator as two line segments, instead of one, in order that each (of the 8) line segments have the same length.

You are asked to address the following issues:

1. Write a code to generate the corners of the quadratic Koch fractal for a given level ℓ as described above. Assume that the starting structure (at $\ell = 0$) is a square of sides L . Make a few graphs of the structure for levels, say, $\ell = 2$ and $\ell = 3$, or others, and include them in your report. Make sure that this fractal generator is correct since everything that follows will rely on it. For purpose of comparison, a high resolution image of part of the structure can be found here.

2. Define a *square* lattice of lattice constant, δ , so that the corners of the fractal for any level $\ell \leq \ell_{\max}$ *always* will fall onto a grid point. Note that this means that the lattice constant δ can not be chosen completely independently of L . For the grid that you define, determine which of its points are inside the fractal structure (and which are not).

Comment: When setting this up, it is beneficial to realize that below you are asked to calculate eigenmodes by a finite difference scheme that requires the knowledge of neighboring points and if they are inside the fractal or not. You may therefore benefit from taking this into consideration when designing your data structure.

3. Assume now that we make a fractal drum; that is, the fractal shape is cut out of a thin metal plate and an elastic membrane is spanned over the “fractal” hole in it (just like in Ref. [4]). Let Ω denote the region (of \mathbb{R}^2) covered by the hole and let $\partial\Omega$ represent its boundary (or perimeter).

Quickly study the experimental and numerical results obtained by Sapoval et al. [4], but disregard the numerical method used in this paper since we will adopt a rather different method.

Any oscillation of the membrane (in Ω) is determined by the wave equation $\nabla^2 u = (1/v^2)\partial_t^2 u$ (v is a velocity) subjected to boundary condition $u = 0$ for all times on $\partial\Omega$ (Dirichlet boundary conditions). Fourier transforming the wave equation over time leads to the so-called *Helmholtz equation*

$$-\nabla^2 U(\mathbf{x}, \omega) = \frac{\omega^2}{v^2} U(\mathbf{x}, \omega), \quad \text{in } \Omega \quad (5a)$$

$$U(\mathbf{x}, \omega) = 0 \quad \text{on } \partial\Omega, \quad (5b)$$

where ω denotes angular frequency (consult the Appendix for additional information). Equation (5a) states that ω^2/v^2 is an eigenvalue, and ω the corresponding *eigenfrequency*, for the negative Laplacian operator ($-\nabla^2$), and the function $U(\mathbf{x}, \omega)$ that satisfies Eq. (5), is the *eigenmode* corresponding to the eigenfrequency ω .

Use a standard (5-point) central finite difference approximation for the Laplacian, that converts Eq. (5) into an eigensystem, and solve it to find the eigenfrequencies and corresponding eigenmodes of the quadratic Koch fractal at some level ℓ .

Produce a table of the 10 *smallest* (or more) eigenfrequencies ω/v of the quadratic Koch fractal and make contour plots of the corresponding eigenmodes using units x/L and y/L and superimpose the fractal structure outside which $U(\mathbf{x}, \omega) = 0$. Specify explicitly for which level ℓ your results were obtained.

Check you results by making sure that you can reproduce Fig. 4(a) and Fig. 5 of Ref. [4] (not necessarily using the same level ℓ for the fractal generator).

4. Assume now that you want to investigate the scaling of $\Delta N(\omega)$ with ω . Since $\Delta N(\omega)$ according to Eq.(4) is expected to depend on the properties of the perimeter of the drum, it is of primary interest to use a high level ℓ in the fractal generation. If we want to use, say, $\ell = 8$ or $\ell = 10$, discuss (i) the challenges one faces if using the finite difference approach described above; and (ii) how you can resolve these issues. Note that you are not asked to implement these suggestions, only present a discuss.

5. A problem closely related to the membrane problem considered above, is the vibration modes of a *clamped thin plate*. For a smooth boundary this is a “standard” problem in continuum mechanics. It is outside our scope to describe in detail the mathematical formulation (and derivation) of the problem. More information can be found in Ref. [7], but it will not be needed to solve the problem.

The relevant equations are

$$\nabla^4 W(\mathbf{x}, \omega) = \lambda W(\mathbf{x}, \omega) \quad \text{in } \Omega \quad (6a)$$

$$W(\mathbf{x}, \omega) = 0 \quad \text{on } \partial\Omega \quad (6b)$$

$$\partial_n W(\mathbf{x}, \omega) = 0 \quad \text{on } \partial\Omega, \quad (6c)$$

with the normal derivative defined as $\partial_n = \hat{\mathbf{n}} \cdot \nabla$ where $\hat{\mathbf{n}}$ is the outward normal vector to the boundary. The operator $\nabla^4 = \nabla^2 \nabla^2$ is known as the biharmonic operator so that Eqs. (6) represent the *biharmonic eigenvalue problem* with homogeneous Dirichlet boundary conditions.

Find the few lowest eigenvalues and corresponding eigenmodes for this biharmonic eigenvalue problem. Compare your results to those of the vibrating membrane problem considered under point 3.

Note that except for the Laplace operator being replaced by the biharmonic operator and an additional boundary condition, this problem is similar to the one that you solved above. *Hint*: Before coding anything, make sure you understand the implications of the extra boundary condition.

6. (*Optional*) We now revisit the vibrating membrane problem (task 3). For extra credit (only to be considered if you have finished *all* the other tasks), you are asked to investigate the scaling of $\Delta N(\omega)$ for an as high level ℓ that is practically possible with your implementation (and available computer resources). Can you obtain any estimates for d ?

A Some extra material

We start with a motivation section for studying the eigenvalue problem of the Laplace operator with Dirichlet boundary conditions on an arbitrary domain. You may recognize in the motivation section some notions you have probably seen elsewhere. If not, we hope to give a feeling about the interest one has in solving the eigenvalue problem of the Laplace operator. In either case, you will not need to understand in great details this first section in order to work on the problem and therefore should not spend too much time reading this motivation section.

A.1 Motivation

We consider Ω a domain of \mathbb{R}^n , of boundary $\partial\Omega$. Let $u(\mathbf{x}, t)$ denote a function depending on a time variable t and space variables \mathbf{x} . Imagine we are interesting in solving one of these equations of physical interest on this domain,

the diffusion equation:

$$\frac{\partial u}{\partial t} = D \nabla^2 u \quad (7)$$

the wave equation:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u \quad (8)$$

the Schrödinger equation:

$$i\hbar \frac{\partial u}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 u \quad (9)$$

given some initial conditions,

$$u(0, \mathbf{x}) = u_{\text{in}}(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega, \quad (10)$$

$$\frac{\partial u}{\partial t}(0, \mathbf{x}) = v_{\text{in}}(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega, \text{ (for the wave equation)} \quad (11)$$

with Dirichlet boundary conditions

$$u(\mathbf{x}, t) = 0, \quad \forall \mathbf{x} \in \partial\Omega. \quad (12)$$

You are most probably familiar with these equations, but we recall the possible physical meaning of each of them. The diffusion equation could model here the diffusion of a chemical, or of temperature in a medium, with absorbent boundaries. The wave equation models the vibrations of a membrane ($n = 2$) which has been stretched and fixed at the boundary, like a drum for example. The Schrödinger equation describes the evolution of the wave function of a free particle in a box, the domain Ω .

It is worth noting the presence of the Laplace operator $\nabla^2 u = \sum_{i=1}^n \frac{\partial^2 u}{\partial x_i^2}$ in all these cases. This is a key observation that can be used to solve simultaneously the three above problems, as we motivate now.

Assume that we are looking for solutions of the form

$$u(\mathbf{x}, t) = \phi(t) w(\mathbf{x}), \quad (13)$$

then by plugging Eq. (13) into Eqs. (7), (8), and (9) we get, at least formally,

for the diffusion equation:

$$\frac{1}{D} \frac{\phi'}{\phi} = \frac{\nabla^2 w}{w}, \quad (14)$$

for the wave equation:

$$\frac{1}{c^2} \frac{\phi''}{\phi} = \frac{\nabla^2 w}{w}, \quad (15)$$

for the Schrödinger equation:

$$\frac{2m}{i\hbar} \frac{\phi'}{\phi} = \frac{\nabla^2 w}{w}. \quad (16)$$

In each of these last three equations, the left hand side is a function of time only and the right hand side is a function of position only. The only way this can hold for any time and at any position, is that both the left and right hand sides are constant, say $-\lambda$, with $\lambda \in \mathbb{R}$. Note that λ is an unknown. The convention for the minus sign will become clear below. Thus we must have

$$\frac{\phi'}{\phi} = -D \lambda \text{ or } = -\frac{i\hbar}{2m} \lambda, \quad (\text{Diffusion and Schrödinger equations}) \quad (17)$$

$$\frac{\phi''}{\phi} = -c^2 \lambda, \quad (\text{Wave equation}) \quad (18)$$

and

$$-\nabla^2 w = \lambda w. \quad (19)$$

Equations (17) and (18) can be integrated simply as

$$\phi(t) = \phi_0 \exp(-D \lambda t) \text{ or } = \phi_0 \exp\left(-\frac{i\hbar}{2m} \lambda t\right), \quad (\text{Diffusion and Schrödinger equations}) \quad (20)$$

$$\phi(t) = A \exp\left(i c \sqrt{\lambda} t + \varphi_0\right), \quad (\text{Wave equation}). \quad (21)$$

We recognize the usual time dependencies for the diffusion equation and wave equations, namely an exponential decay in time for the first one and vibrations for the second one. If you are familiar with Quantum Mechanics, you will also recognize the time evolution phase factor $\exp(-i \frac{E}{\hbar} t)$ depending on energy $E = \frac{\hbar^2 \lambda}{2m}$.

Now, the only problem that remains to be solved is the eigenvalue problem Eq. (19), i.e. finding the eigenvalues and corresponding eigenfunctions of the Laplace operator satisfying the boundary conditions. If we manage to find the eigenvalues $(\lambda_k)_{k \in \mathbb{N}}$ and corresponding eigenfunctions $(w_k)_{k \in \mathbb{N}}$ then we can expand the initial condition u_{in} on the basis of eigenfunctions and apply the corresponding time dependency. For example, in the case of the diffusion, if the expansion of the initial condition on the basis of eigenfunctions reads

$$u_{\text{in}} = \sum_k \alpha_k w_k, \quad (22)$$

then the solution is immediately given by

$$u(\mathbf{x}, t) = \sum_k \alpha_k e^{-D \lambda_k t} w_k(\mathbf{x}). \quad (23)$$

You recognize here something that we have used in assignment 2 when we compared the numerical solution of the 1-dimensional diffusion equation $n = 1$ with exact solutions on a bounded domain which had the form Eq. (23).

To sum up this motivation section, we can say that the three problem we started with can be solved once and for all if we manage to find the eigenvalues and eigenfunctions of the Laplace operator that satisfy the appropriate boundary conditions. In fact, this is in general the hard part of the problem, since in practice the boundary may be of arbitrary shape, which makes the resolution of the eigenvalue problem challenging.

Note that the eigenfunctions, also known as eigenmodes, are not simply mathematical commodities but also have a physical meaning. If we take the example of the two-dimensional drum, the eigenmodes are modes of resonant frequencies of the membrane.

In the following, we will restrict ourselves to a two-dimensional domain, and it may be helpful to think of the problem as finding the resonant modes of a drum with arbitrary shapes.

A.2 A simple example: rectangular domain

We consider the eigenproblem of the Laplace operator with Dirichlet boundary conditions. The domain $\Omega = (0, L_x) \times (0, L_y)$, with $L_x, L_y > 0$, is a rectangle and the problem reads

$$-\nabla^2 u = \lambda u, \quad \text{in } \Omega \quad (24)$$

$$u = 0, \quad \text{on } \partial\Omega \quad (25)$$

where u is a function of position (x, y) .

We can show that the eigenvalues and corresponding eigenmodes of the above problem read, for $k = (k_x, k_y) \in \mathbb{N}_*^2$,

$$\lambda_k = \frac{k_x k_y \pi^2}{L_x L_y}, \quad (26)$$

$$u_k(x, y) = 2 \sin\left(\frac{k_x \pi x}{L_x}\right) \sin\left(\frac{k_y \pi y}{L_y}\right). \quad (27)$$

References

- [1] Assignment no 2 can be found here.
- [2] M. Kac, *Can One Hear the Shape of a Drum?*, American Mathematical Monthly **73**, 1–23 (1966). Downloadable version.

- [3] Wikipedia page: “Hearing the shape of a drum”.
- [4] B. Sapoval, T. Gobron, and A. Margolina, *Vibrations of fractal drums*, Phys. Rev. Lett. **67**, 2974–2977 (1991). Downloadable version.
- [5] S. Homolya, *Generalisation of the modified Weyl-Berry conjecture for drums with jagged boundaries*, Phys. Lett. A **318**, 380–387 (2003). Downloadable version.
- [6] C. Hua and B.D. Sleeman, *Fractal Drums and the n-Dimensional Modified Weyl-Berry Conjecture*, Commun. Math. Phys. **168**, 581–607 (1995). Downloadable version.
- [7] Wikipedia page: “Vibration of plates”.