EXAMPLES CLASS IN MATHEMATICAL PHYSICS

II. Eigenfunction Expansions and Fourier Analysis (2.12.98)

Commentary: This sheet concerns the solution of linear differential equations in physics by expansion in normal modes (eigenfunctions). In many cases the expansion turns out to be some sort of Fourier series.

Normal mode (eigenfunction) analysis plays a central role in several parts of the physics course. Typically an eigenfunction is a function of a continuous variable (for instance a spatial coordinate) and there are correspondingly an infinite set of normal modes, whose completeness and orthogonality can be exploited in calculating the time evolution of the system. In section A we examine the time evolution of a stretched string.

Normal mode analyses are equally important when studying systems with a finite number degrees of freedom. This includes the quantum physics of spin systems (introduced in the problem sheets of the quantum course). An example of a system whose behaviour can be described by only two normal modes is worked through in Section B, though in this case the system involves a brewery rather than anything quantum mechanical.

Section C returns to continuous systems - an application of eigenfunction analysis to an important equation of classical physics, the heat diffusion equation. We then establish a formal connection between Fourier Analysis and eigenfunction expansions by introducing a special choice of boundary conditions.

Several of the questions are as much exercises in getting the algebra right as exercises in physics. This is something every practising physicist has to be able to do!

A. Eigenfunction Expansions

A1. Eigenfunctions. Subject to given boundary conditions (which *must* be specified), a self-adjoint (Hermitian) operator, H, has a *complete* set of *orthogonal* eigenfunctions, $\phi_n(x)$:

$$H\,\phi_n(x) = E_n\,\phi_n(x)\ . \tag{1}$$

Assuming the ϕ_n to be normalized, the orthogonality condition is

$$\int \phi_m^*(x)\phi_n(x)dx = \delta_{mn}\ . \tag{2}$$

Any function $f(x)$ can then be expanded in terms of the complete set of eigenfunctions:

$$f(x) = \sum_n c_n\phi_n(x) \tag{3}$$

where

$$c_m = \int \phi_m^*(x)f(x)dx\ . \tag{4}$$

[If you are unsure of this equation, prove it by substitution of (3) in (4) and using (2).]

A2. Vibrations of a stretched string. Recall from your waves course that the equation of motion of a string under tension T and of lineal density ρ is

$$\frac{\partial^2\psi}{\partial t^2} = c^2\frac{\partial^2\psi}{\partial x^2} \tag{5}$$

where $c = \sqrt{(T/\rho)}$ is the velocity of wave propagation along the string and $\psi(x,t)$ is the displacement.

For a string stretched between $x = 0$ and $x = L$ possible boundary conditions (BC's) include:

(a) Dirichlet BC's: eigenfunctions go to zero at the boundaries of the box;

(b) Neumann BC's: first derivatives vanish: $\psi'(0) = 0, \psi'(L) = 0$;

(c) Periodic BC's: the eigenfunctions are periodic with period L;

or a mixture of these. Finding the BC's appropriate to a given physical situation is an important part of setting up the problem in mathematical terms. Give a physical example of (b) for a string.

(i) We shall consider a string fixed at $x = 0$ and $x = L$. What are the boundary conditions?

(ii) Find the *normal modes of vibration* of the string, taking into account the boundary conditions of the problem. In other words, confirm that a complete set of separable solutions is of the form $\phi_n(x,t) = \phi_n(x)\exp(-i\omega_n t)$. Insertion into (5) gives an equation of the form (1), a "time independent wave equation" where the operator H takes the form $-c^2\frac{\partial^2}{\partial x^2}$. Confirm that, for the boundary conditions we have taken, the spatial part of the normalised eigenfunctions is

$$\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad , \quad n = 1, 2, 3... \tag{6}$$

What are the corresponding frequencies of oscillation of the normal modes?

(iii) Use the results of Section A1 to show that any (see note on page 8) real function $f(x)$, defined on the interval $0 < x < L$, can be expanded as follows:

$$f(x) = \sum_{n=1}^{\infty} a_n \, \sin\left(\frac{n\pi x}{L}\right) \tag{7}$$

$$a_n = \frac{2}{L}\int_0^L f(x)\, \sin\left(\frac{n\pi x}{L}\right) dx \tag{8}$$

These equations resemble ones you will have seen in the theory of Fourier analysis; the similarity is no accident.

A3. The time evolution problem.

The importance of eigenfunctions in the study of differential equations in physics stems from the fact that their time-dependence is simple. A specified initial condition can be decomposed into eigenfunctions, these evolved according to simple rules, and the behaviour at a later time synthesized be superposing the time-evolved functions. The method is quite general and is employed in many problems such as quantum mechanics, heat conduction, diffusion, and wave motion. Some of these applications are given in subsequent sections.

Consider the following problem:

"A string under tension T and of length $2L$ is initially clamped at its midpoint $x = L$ and the section $(0, L)$ is oscillating with unit amplitude in its fundamental mode $n = 1$. The section $(L, 2L)$ is at rest. At time $t = 0$, when the section $(0, L)$ is at the maximum of its displacement (and therefore momentarily at rest), the clamp is suddenly removed. What is the subsequent motion of the string?"

To solve this:

(i) Sketch the initial displacement.

[Ans: $\psi(x, 0) = \sin\left(\frac{\pi x}{L}\right), \quad 0 < x < L;\ \psi(x, 0) = 0 \quad , L < x < 2L.$]

(ii) Use (7) to write $\psi(x, 0)$ as a sum over the eigenfunctions $\phi_n(x)$ of the new (longer) string, and find the coefficients a_n. To simplify this procedure, first show that $a_n = 0$ for all even n except $n = 2$; then calculate a_2. Also, you may use without proof the following formula which applies for n odd:

$$\int_0^L \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{n\pi x}{2L}\right) dx = \frac{L}{\pi}(-1)^{(n+1)/2} \frac{4}{n^2 - 4} \quad . \tag{9}$$

(iii) What are the frequencies governing the time evolution of the new eigenfunctions of the string $(0, 2L)$?

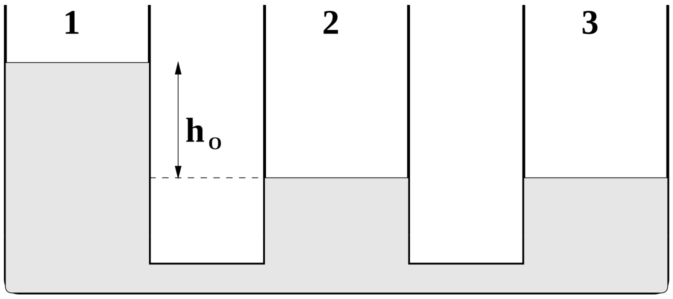
(iv) Hence obtain a general expression for $\psi(x, t)$ at times $t > 0$.

[Ans.: $\frac{1}{2} \sin\left(\frac{\pi x}{L}\right) e^{-\frac{ic\pi}{L}t} + \sum_{n=1,3,5...} \frac{4}{\pi} \frac{(-1)^{(n+1)/2}}{n^2-4} \sin\left(\frac{n\pi x}{2L}\right) e^{-\frac{icn\pi}{2L}t}$.]

B. Systems with few normal modes

The problem just considered involved an infinite number of eigenfunctions. There are some quantum problems (those involving spin systems, for example) and many classical ones, where only a few degrees of freedom are involved. Here is one example:

B1. A problem with beer. "A brewery contains three identical large cylindrical vats of constant cross-section, connected by two similar small pipes as shown in the figure. Initially the fluid level in vat 1 exceeds that of the other two vats by an amount h_0. Find the maximum amount by which the height in vat 2 exceeds that in vat 3 at subsequent times. You may assume that the liquid is incompressible and the flux of liquid through each pipe is proportional to the pressure difference across it."



To solve this problem, we must first define our variables. We could use the heights of liquid in each of the tanks, but only two of these are independent (as the total volume of liquid is constant). So it is better to define $h_1(t)$ as the amount by which the level of fluid in vat 1 exceeds that in vat 2, and $h_2(t)$ as the amount by which that in vat 2 exceeds that in vat 3. It is then convenient to represent the state of the system as a 2-component vector $\mathbf{h} = (h_1, h_2)$ which depends on time.

(i) The next step is to find the equations of motion. The pressure differences across the two pipes are proportional to h_1 and h_2 respectively (why?). Denoting the volumes of liquid in the vats by $V_{1,2,3}$, we therefore have (with c some constant)

$$\dot{V}_1 = -ch_1 \ \ ; \ \ \dot{V}_2 = c(h_1 - h_2) \ \ ; \ \ \dot{V}_3 = ch_2 \ \ .$$

We also know that $Ah_1 = V_1 - V_2$ and $Ah_2 = V_2 - V_3$, where A is the cross section of the vats. Use these results to obtain the equations of motion in the matrix form (where the constant $\mu = c/A$):

$$\begin{pmatrix} \dot{h}_1 \\ \dot{h}_2 \end{pmatrix} = \begin{pmatrix} -2\mu & \mu \\ \mu & -2\mu \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \end{pmatrix}$$

(ii) Find the eigenvectors $\mathbf{v}_1$, $\mathbf{v}_2$ and eigenvalues λ_1, λ_2 of the matrix. Show that there are separable solutions of the form $\mathbf{h}(t) = \mathbf{v}_1 f_1(t)$ and $\mathbf{h}(t) = \mathbf{v}_2 f_2(t)$ and find $f_1(t)$ and $f_2(t)$. What is the time-dependence of the height vector $\mathbf{h}$ starting from (a) an initial condition in which h_1 and h_2 are equal; (b) when they are opposite?

(iii) The initial condition in the problem as given is $(h_1, h_2) = (h_0, 0)$. Write this as a superposition of the two eigenvectors with appropriate coefficients. Since the equations of motion are linear in the h's, these two eigencomponents evolve independently as found in (ii). Exploit this fact to give the complete solution for $h_1(t)$ and $h_2(t)$ at later times t. Sketch curves for both of these on the same axes, and interpret your results physically.

[Ans: $h_1 = \frac{1}{2}h_0(e^{-\mu t} + e^{-3\mu t}); h_2 = \frac{1}{2}h_0(e^{-\mu t} - e^{-3\mu t})$]

(iv) To complete the problem as asked, calculate the maximum value of $h_2(t)$.

[**Remark:** This question is based on one in a recent Part II Physics and Theoretical Physics examination (the general physics paper). Notice how a method taught in these examples classes can dramatically reduce the work involved.]

C. Eigenfunctions vs. Fourier Series

C1. Consider the **heat diffusion equation** in one dimension

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}$$

where $\kappa = K/C\rho$, K being the thermal conductivity, ρ the density and C the specific heat capacity of the material.

A thin iron rod ($\kappa = 5 \times 10^4$ m^2 s-1) is heated unevenly and then thermally insulated and left to reach equilibrium. It extends from $x = -a$ to $x = a$, where the length $2a$ of the rod is 0.1m. At time zero, the half of the rod $-a < x < 0$ is at 100 degC and the other at 0 degC.

(i) What are suitable boundary conditions at the ends of the rod? [Hint: Consider the heat flux, which is given by $K\partial T/\partial x$.]

(ii) What are the eigenfunctions? Sketch the first four.

(iii) Find the general solution as a function of time. Check that the final steady state limit is what you would expect on physical grounds, for an insulated bar whose average initial temperature is 50 degC. [If it disagrees, check you did not forget the lowest eigenfunction in (ii).]

(iv) Write down an approximate formula that describes the approach to this steady state solution in the limit of long times. [Ans.: $T(x,t) \simeq 50 - \frac{200}{\pi} \sin\left[\frac{\pi x}{2a}\right] \exp\left[-\frac{\pi^2 \kappa t}{4a^2}\right]$.]

(v) Use this to find how long must elapse before the ends of the rod reach 52 degC and 48 degC. In what sense is this a "long" time?

C2. Fourier's Theorem. Imagine we have a function $f(x)$ which is periodic with period L:

$$f(x+L) = f(x)\ .$$

This can be expanded in terms of any complete set of orthogonal functions with the same period. One choice is the set of complex exponentials, in terms of which *Fourier's theorem* (in its complex form) states that:

$$f(x) = \sum_{-\infty}^{\infty} a_n e^{i2\pi nx/L}$$

$$a_n = \frac{1}{L}\int_0^L f(x)\, e^{-i2\pi nx/L}\ .$$

These equations also have another interpretation. Suppose we take just one period of the function, $f(x)$ in the range $0 < x < L$, and expand it in terms of the eigenfunctions of a stretched string, under the following choice of boundary conditions:

$$\phi(0) = \phi(L)$$

$$\phi'(0) = \phi'(L) \ .$$

These are often known as *periodic boundary conditions*.

(i) Can you see why they ensure that all the eigenfunctions are periodic?

(ii) Confirm that the normalized eigenfunctions may be chosen as

$$\phi_n(x) = \sqrt{\frac{1}{L}} e^{i2n\pi x/L} \quad , \quad n = 0, \pm 1, \pm 2, ...$$

where n now runs over both positive and negative values.

(iii) Show that Fourier's theorem as defined above is a special case of (3) and (4).

(iv) Chemists sometimes use the one dimensional particle-in-a-box problem (with Dirichlet BC's) to model the electron energy levels of a linear polymer molecule such as polyethyne. Can you think of a similar physical problem for which the periodic BC's would instead be appropriate?

NOTES: (1) Because all the eigenfunctions have the same period as f, the expansion is valid even outside the original interval $0 < x < L$. This would not be true if we expanded in, say, the closed box eigenfunctions used in Q.A2.

(2) Fourier's theorem for periodic functions can also be written as an expansion in terms of a set of real eigenfunctions (sines and cosines). These eigenfunctions may be constructed by superposing pairs of complex exponentials of equal and opposite n, which are degenerate in energy. The corresponding result is $f(x) = b_0/2 + \sum_{n=1}^{\infty} \left[a_n \sin\left(\frac{2n\pi x}{L}\right) + b_n \cos\left(\frac{2n\pi x}{L}\right)\right]$ where $a_n = \frac{2}{L}\int_0^L f(x) \sin\left(\frac{2n\pi x}{L}\right) dx$ and $b_n = \frac{2}{L}\int_0^L f(x) \cos\left(\frac{2n\pi x}{L}\right) dx$; this should also be a familiar form of Fourier's theorem.

(3) Remarks to eqtn. (7). If the function to be expanded satisfies the same boundary conditions as the complete set used to expand it, then one gets the correct expansion at

all points. If it satisfies different boundary equations, then the expansion is correct at all points in the interval excluding the end points.