

Matematisk Fysik

Paolo Sibani
Institut for Fysik og Kemi, SDU

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Chapter 1

Introduction

Fysik 505 is a hands-on course on linear algebra, where selected examples are analyzed using mathematical tools and a numerical software package called Matlab. We also discuss the physics behind the examples, learning how the same mathematics can be given different interpretations.

The approach is ‘learning by doing’, which means that active participation is required in order for you to benefit from the course. This means *interacting* with your fellow students, with your teacher(s) and with the computer. Please do not be afraid to *ask questions*, either directly or by e-mail.

Specifically about these notes and how to use them:

I have not attempted to write a book. Many books are available and can be consulted for more details, better arguments etc.

As you work through the chapters, you should document your progress by writing a log-book, which contains your thoughts, calculations, figures etc. The log-book can be used as raw material for writing a report.

In the final report you should attempt to argue your case. Why should you, the examiner, or anybody else trust the results? This is an important step usually neglected in introductory courses.

Chapter 2

Matlab primer

Target

The purpose of this session is to get you acquainted with basic MATLAB commands, functions and plotting tools, while trying your hand at simple problems of linear algebra.

Method

This first session, most of the code you need is given below. You will need to understand its structure and play with it in order answer some basic questions.

Simple manipulations

The following three exercises relate to basic MATLAB operations.

1. The *help* command gives you access to a well-structured on-line manual for Matlab. You can also invoke the command with an argument, e.g. *help linspace*.
2. Using the help function, familiarize yourself with *linspace*. With *linspace*, create an array *t* of time values equally spaced from 0.1 to 10. The length of the array should at least ten values.
3. Neglecting friction, the vertical displacement of a freely falling object is $dS = \frac{1}{2}gt^2$, where $g \approx 10\text{ms}^{-2}$. Using this formula, create an array *dS* containing the values of the displacement at the times given in *t*.

4. Learn about the command *plot*, and use it to plot dS versus t on a linear and a log-log scale.
5. Plot the graph of a function $f(x)$ of your choice for values of x in the unit interval.

Vector space concepts in Matlab

A vector in an M dimensional complex vector space can be represented as an array of M complex numbers. The standard basis consists of M column vectors \mathbf{e}_j , $j = 1, 2, \dots, M$ where $\mathbf{e}_j(k) = \delta_{jk}$. The symbol δ_{jk} , called Kronecker delta, stands for a function of two integer arguments. The function vanishes for $k \neq j$ and equals one if $k = j$.

Consider now the following MatLab example:

Standard basis

```
>> M=3;
>> d = linspace(1,1,M)

d =
     1     1     1

>> E = diag(d,0)
E =
     1     0     0
     0     1     0
     0     0     1

>> E(:,2)
ans =
     0
     1
     0
```

The j 'th column of the matrix E can be extracted by the command $E(:,j)$. The three columns of E constitute a standard basis for \mathbb{C}^3 .

Matrix multiplication

A matrix with n rows and l columns is called an $n \times l$ matrix. Important special cases are a *row vector*, which is a $1 \times l$ matrix, a *column vector*, which is an $l \times 1$ matrix, and a square matrix, where $n = l$.

```
>> a = [1 1 0; 2 0 1; 3 3 3]
a =
     1     1     0
     2     0     1
     3     3     3
```

is an example of a 3×3 matrix.

Inner product

The inner product (a, b) of two vectors a and b is a scalar. The operation is done in Matlab by multiplying a *row* vector with a *column* vector.

```
>> a = [1; 0; 5]
a =
     1
     0
     5
>> b = [0 2 -1]
b =
     0     2    -1
The inner product is:
>> b*a
ans =
    -5
```

We can think of a *row* vector b as a linear mapping of \mathbb{C}^3 into \mathbb{C} .

$$b : a \rightarrow b \cdot a$$

The mapping projects a into the direction of b and scales the result with the length of b .

Outer product of two vectors

From two vectors a and $b \in \mathbb{C}$, one can construct the linear mapping $r \rightarrow a(b, r)$. The mapping is called the outer or tensor product of a and b . The corresponding matrix in the standard basis is easily obtained in Matlab:

```
>> a*b
ans =
     0     2    -1
     0     0     0
     0    10    -5
```

Importantly, the 'multiplication' sign has a **context dependent meaning**. I.e. $b * a$ and $a * b$ are different mathematical objects. Sometimes multiplication (or another operation) is meaningless. If so, Matlab will let you know:

```
>> b*b
??? Error using ==> mtimes
Inner matrix dimensions must agree.
```

Matrix multiplication $a * b$ is only defined when the number of columns in a equals the number of rows in b .

Pointwise operations

Whenever an identical operation must be performed on each component of a vector, one can use 'pointwise' operations, using an arithmetic operator preceded by a dot. The following example shows pointwise multiplications of the elements of b :

```
>> c=b.*b
c =
     0     4     1
```

The `.*` replaces the loop

```
>> for k=1:3
c(k) = b(k)*b(k);
end
```

Loops are computationally inefficient and should be avoided in Matlab whenever possible.

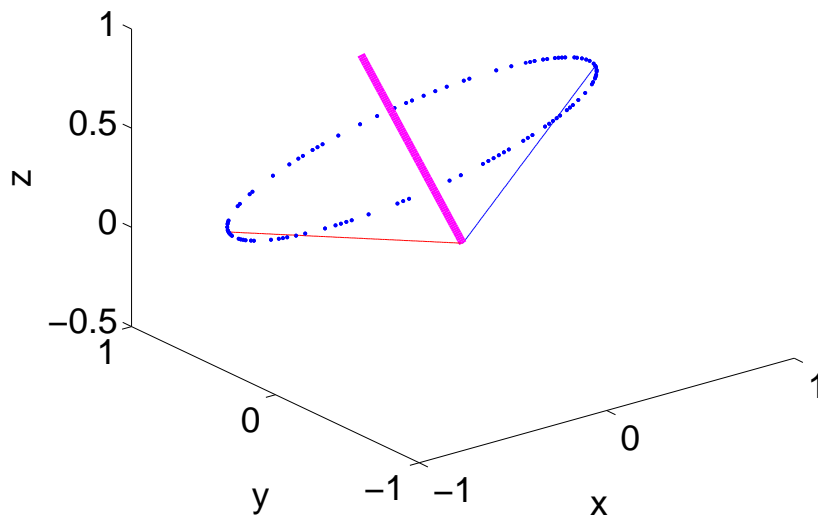


Figure 2.1: The figure is obtained using Eq. 2.2. The thick axis is the rotation axis.

Linear operations on vectors

A linear mapping A is fully determined by its action on a basis, e.g. the standard basis $\{\mathbf{e}_k\}$. In a given basis, the mapping is represented by a matrix, with elements

$$A_{kl} = (\mathbf{e}_k, A\mathbf{e}_l). \quad (2.1)$$

We now consider rotations in 3D as an important example of linear mappings. A rotation R is a linear operation, or better, a linear *operator* characterized by a rotation axis $\hat{\mathbf{n}}$, and a rotation angle ϕ . A coordinate-free way to represent a rotation in 3D is

$$R(\mathbf{r}) = \mathbf{r} + \hat{\mathbf{n}} \times (\hat{\mathbf{n}} \times \mathbf{r})(1 - \cos(\phi)) + \hat{\mathbf{n}} \times \mathbf{r} \sin(\phi), \quad (2.2)$$

where \times indicates the cross product.

1. How many real numbers do you need to specify a rotation in 3D?

2. The matlab program *rotate.m* produces Fig. 2.1. Modify the program to produce similar figures with different rotation axes.
3. Choose a rotation axis parallel to the z axis, and find the matrices of the linear operators $\hat{\mathbf{n}} \times (\hat{\mathbf{n}} \times (\cdot))$ and $\hat{\mathbf{n}} \times (\cdot)$ in the standard basis. To find the matrix elements, you can apply Eq. 2.1.
4. What is the matrix of R in the same basis?
5. Find the eigenvalues of this matrix. Hopefully, one eigenvalue will be equal to one. Give a physical interpretation of the corresponding eigenvector.
6. What is the matrix of R^2 in the same basis? Give a geometrical interpretation of R^2 .
7. Let $\phi = \frac{\pi}{4}$. Using Matlab, find the vector r which solves the equation

$$Rr = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \quad (2.3)$$

Consider now a reflection S in the $x - y$ plane.

1. Write down the matrix for S in the standard basis.
2. Find the eigenvalues of S and interpret these geometrically.

Chapter 3

Stochastic matrices

Target

The purpose of this session is to get you acquainted with basic matrix operations using a particular class of matrices called *stochastic matrices*.

An example

Every month, a statistics is compiled for how many new cars of type i , $i = 1, 2 \dots N$ are bought by customers who turn in a used car of type j , $j = 1, 2 \dots N$. If, for example, $i = 1$ means Volkswagen and $j = 5$ means Toyota, $n_{5,1}$ is the number of customers trading in a used Volkswagen for a new Toyota, and, conversely, $n_{1,5}$ is the number of those trading in an old Toyota for a new Volkswagen. Dividing by the total number of purchases of new cars of type i one estimates the probability $W_{i,k}$ that a car of type k is traded in for a new one of type i . Assuming that a person selling a car of type k buys a new car with probability one, we obtain the normalization condition

$$\sum_{i=1}^N W_{i,k} = 1. \quad (3.1)$$

The above considerations lead us to the following useful definition: A stochastic matrix is a square matrix having non-negative entries and column sums all equal to one.

Returning to our example, a fraction $p(1, i)$ of the cars on the market is of type i in the first month of the year. Every month the fraction changes to a new value, i.e. $p(n, i)$ after n months of trading.

Mathematical manipulations

The following exercise relates matrix operations to basic concept of probability theory..

1. Show that

$$p(n+1, i) = \sum_{k=1}^N W_{i,k} p(n, k). \quad (3.2)$$

2. Argue that the operation can conveniently be written in matrix notation as the multiplication

$$\mathbf{p}(n+1) = \mathbf{W}\mathbf{p}(n) \quad (3.3)$$

where \mathbf{W} is a stochastic $N \times N$ matrix with elements $W_{i,j}$ and $\mathbf{p}(n)$ is a column vector (a $N \times 1$ matrix), describing the distribution of car types owned after n months.

3. Show that if \mathbf{A} and \mathbf{B} are stochastic matrices, their product $\mathbf{C} = \mathbf{A}\mathbf{B}$ is stochastic. Is the same true for their sum and difference $\mathbf{A} \pm \mathbf{B}$?
4. Argue that after n months the distribution of car types is

$$\mathbf{p}(n+1) = \mathbf{W}^n \mathbf{p}(1). \quad (3.4)$$

Matlab knee-bends

The following matlab script would not earn you high marks in a project assignment.

```
clear
N = 5; %number of car types
tmax = 10;
w = zeros(5); % a square zero matrix
for k=1:N
x = rand(N,1);
x = x/sum(x); %normalization of columns
w(:,k) = x;
end
```



```
p = rand(5,1);
p = p/sum(p); %initial car distribution
tr = p;
for k=1:tmax
    p = w*p;
    tr = [tr p];
end %what happens in the loop ?
plot(tr');
hold on
plot(tr', '*');
hold off %not (yet) a good plot.
```

1. Make sure you understand what the variables mean and what the operations appearing in the script do.
2. Correct the plot so that it clearly appears what is plotted as a function of what. Then comment the different curves.
3. Compare the eigenvalues of the matrix \mathbf{w} with those of \mathbf{w}^n , where n is a sufficiently large integer. What are your thoughts?

Chapter 4

Coupled differential equations

Target

Here we introduce a set of coupled differential equations which describe the time evolution of a set of particles diffusing on a set of M point arranged in a linear array. This set of occupation numbers $\{n(j, t)\}$ can be considered as an element in an M dimensional vector space.

Coupled ODE's. A simple example

We consider a linear array of 'sites' $i = 1, 2 \dots M$. On each of these sites a number of particles can reside. Let $n(i, t)$ be the number of particles on site i . In the model, the particles can hop to their nearest neighbor at rate $1/\tau$.

Let us first consider sites away from the boundary sites $i = 1$ and $i = M$. On these internal sites

$$\tau \frac{dn(j, t)}{dt} = n(j - 1, t) + n(j + 1, t) - 2n(j, t), j = 2, \dots M - 1. \quad (4.1)$$

What happens at the boundary depends on the *boundary conditions*. We consider:

Absorbing boundaries : In this case nothing flows into site 1 and M from the left, respectively right, and particles flowing out never return. The corresponding equations are

$$\tau \frac{dn}{dt}(1, t) = n(2, t) - 2n(1, t) \quad (4.2)$$

$$\tau \frac{dn}{dt}(M, t) = n(M - 1, t) - 2n(M, t). \quad (4.3)$$

Reflecting boundaries : In this case, nothing flows in or out of the system, and

$$\tau \frac{dn}{dt}(1, t) = n(2, t) - n(1, t) \quad (4.4)$$

$$\tau \frac{dn}{dt}(M, t) = n(M - 1, t) - n(M, t). \quad (4.5)$$

Periodic boundaries : In this case we do away with the boundaries by considering a circular array of points. Then, particle exiting at the right re-enter at the left end and vice-versa.

$$\tau \frac{dn}{dt}(1, t) = n(M, t) + n(2, t) - 2n(1, t) \quad (4.6)$$

$$\tau \frac{dn}{dt}(M, t) = n(M - 1, t) + n(1, t) - 2n(M, t). \quad (4.7)$$

Writing the tuple $n(1, t), \dots, n(M, t)$ as the column vector $\mathbf{n}(t)$, all above equations can be written as

$$\tau \frac{d\mathbf{n}}{dt} = \Delta^2 \mathbf{n} \quad \text{or, equivalently} \quad (4.8)$$

$$\frac{d\mathbf{n}}{dt} = T \mathbf{n}. \quad (4.9)$$

Δ^2 is the lattice Laplacian, and T is the same, except that it incorporates for convenience the time constant τ : $T = \frac{\Delta^2}{\tau}$. Δ^2 can easily be defined for any type of regular lattice, and even for a arbitrary connected graphs.

T is an $M \times M$ matrix, whose form depends in certain details on the boundary conditions. The form given in the MatLab script *diff0.m* is for absorbing boundary conditions. The solution of Eq. (4.9) can in all cases be written as

$$\mathbf{n}(t) = \exp(tT) \mathbf{n}_0, \quad (4.10)$$

where \mathbf{n}_0 is the initial distribution of particles.

1. Figure out what the exponential of a matrix means and suggest at least one way to calculate it.
2. Using a suitably modified version of the script *diff0.m*, calculate the total number of particles which remain in the system at time t as a function of t . Also, plot the distribution $\mathbf{n}(t)$ at selected times.

3. Repeat the above for reflecting boundary conditions (NB: you have to modify T).
4. Repeat the above for periodic boundary conditions (NB: you have to modify T once again).

Chapter 5

Eigenvalue problem for the lattice Laplacian

Target

In our second session we learn about the eigenfunctions and eigenvectors of the (lattice) Laplace operator with periodic boundary conditions, and about their relation to Fourier transforms.

Eigenvalue problem for lattice Laplacian

In vector-matrix notation, the ODE considered here and in the previous session has the form

$$\tau \frac{d\mathbf{n}}{dt} = \Delta^2 \mathbf{n}, \quad (5.1)$$

where \mathbf{n} is an M dimensional complex vector and Δ^2 is the lattice Laplacian previously discussed. Eventually, we shall wind up with real-valued solutions, but it is much easier to work with complex valued vectors along the way.

We use the inner product

$$(\mathbf{n}_1, \mathbf{n}_2) = \sum_{j=1}^M \overline{n_1(j)} n_2(j), \quad (5.2)$$

and we let i denote the unit vector along the imaginary axis of the complex plane. Note: the inner product (n_1, n_2) is simply obtained in Matlab using the command:

>> (\mathbf{n}_1')* \mathbf{n}_2

i.e. both transposition and complex conjugation of a complex valued vector are obtained using the apostrophe. The row vector n_1' is called the adjoint of n_1 .

Let $k = 0, 1, \dots, M - 1$, and define, for each k , the M vectors \mathbf{F}_k , with coordinates given by

$$F_k(j) = \frac{1}{\sqrt{M}} \exp(i \frac{2\pi k}{M} j); \quad j = 1, 2 \dots M. \quad (5.3)$$

First some preliminaries:

1. Show that $(\mathbf{F}_k, \mathbf{F}_l) = \delta_{kl}$, where δ_{kl} is the Kronecker's delta.
2. Show that the vectors $(\mathbf{F}_0, \mathbf{F}_1 \dots \mathbf{F}_{M-1})$ are linearly independent.
3. Show that they provide an orthonormal basis for the space \mathbb{C}^M of all complex M dimensional vectors. Find the formula for the coordinates \hat{n}_k of an arbitrary vector \mathbf{n} in this basis.
4. Show that a change from the standard basis to the Fourier basis leaves the inner product unchanged, i.e. :

$$(\mathbf{n}, \mathbf{m}) = \sum_{k=0}^{M-1} \overline{\hat{n}_k} \hat{m}_k \quad (5.4)$$

for any two vectors \mathbf{n} and \mathbf{m} . The overbar denotes complex conjugation.

Now, we bring our ODE into play. We consider periodic boundary conditions.

1. Show that

$$\Delta^2 \mathbf{F}_k = \lambda_k \mathbf{F}_k, \quad (5.5)$$

with the *eigenvalue*

$$\lambda_k = -2 \left(1 - \cos\left(\frac{2\pi k}{M}\right) \right). \quad (5.6)$$

2. Reflect on the mathematical properties of the eigenvalues and eigenvectors of the lattice Laplacian: where do the eigenvalues lie in the complex plane? Can you find degenerate eigenvectors for this problem?

Finally, we solve our ODE using an eigenvalue expansion:

1. We can expand our solution $\mathbf{n}(t)$ in the basis \mathbf{F}_k . The coordinates, $(\mathbf{F}_k, \mathbf{n}(t)) = \hat{n}_k(t)$ are of course functions of time. Show that

$$\hat{n}_k(t) = \hat{n}_k(0) \exp\left(\frac{\lambda_k}{\tau} t\right). \quad (5.7)$$

2. For each of the following two initial conditions:

- (a) $n(0, j) = \delta_{j1}$
- (b) $\mathbf{n}(0) = \mathbf{F}_l$

determine the corresponding values of $\hat{n}_k(0)$, $k = 0, 1 \dots M - 1$.

3. Compare the results obtained with a numerical solution of the ODE.
4. Reflect over the practical and conceptual advantages and disadvantages of using an eigenvalue expansion (in our case a Fourier series) versus using $\exp(tT)$, as was done in the previous session.

Chapter 6

Diffusion & Fourier series

Target

In our third session we consider the heat (or particle) diffusion problem, its connection with the lattice model and its eigenfunctions and eigenvalues. We also learn about the *method of images*.

Eigenvalue problem for the Laplacian

We start again with the discrete problem

$$\tau \frac{d\mathbf{n}}{dt} = \Delta^2 \mathbf{n}. \quad (6.1)$$

We attach to the j 'th point in the lattice the spatial coordinate

$$x_j = j\delta x - L; \quad -L < x_j < L, \quad (6.2)$$

where L is a real number, and where

$$\delta x = \frac{2L}{M}. \quad (6.3)$$

We also treat the j 'th coordinate of \mathbf{n} as a smooth function of space and time $n(x, t)$ taken at the point x_j

$$n(j, t) = n(x_j, t) \quad (6.4)$$

Keeping the value of L fixed, we consider the limit $M \rightarrow \infty$.

1. Justify the approximation $\Delta^2 \approx (\delta x)^2 \nabla^2$, and use this approximation to write Eq. (6.1) as the partial differential equation (PDE)

$$\frac{\partial n}{\partial t} = \frac{(\delta x)^2}{\tau} \nabla^2 n. \quad (6.5)$$

2. The above expression only makes sense if the ratio

$$\frac{(\delta x)^2}{\tau} = D,$$

a so-called diffusion coefficient, remains finite in the limit $\delta x \rightarrow 0$. Discuss the physical meaning of the diffusion coefficient D , and the physical limitations of Eq. (6.5): What happens to the ratio

$$v = \frac{\delta x}{\tau}$$

if D remains finite?

3. It is convenient to have k have values symmetric around zero. Assume that $M/2$ is integer, and let $-M/2 \leq k \leq M/2$. Check the identity

$$n(j') = \sum_{k=-M/2}^{M/2-1} \frac{1}{M} \sum_{j=1}^M e^{\frac{i2\pi}{M} k(j'-j)} n(j), \quad (6.6)$$

and show that it can be written in the limit $M \rightarrow \infty$ as

$$n(x') = \sum_{k=-\infty}^{\infty} \frac{1}{2L} \int_{-L}^L e^{\frac{i\pi}{L} k(x'-x)} n(x) dx. \quad (6.7)$$

This leads to an expression for the complex Fourier coefficient

$$\hat{n}_k = \frac{1}{2L} \int_{-L}^L e^{-\frac{i\pi}{L} kx} n(x) dx, \quad (6.8)$$

with

$$n(x) = \sum_{k=-\infty}^{\infty} e^{\frac{i\pi}{L} kx} \hat{n}_k. \quad (6.9)$$

Show that this agrees with Eq.(6) on Kreyszig page 487.

4. Show that the eigenvalues of Eq. (6.5) approach

$$\frac{\lambda_k}{\tau} \rightarrow -\left(\frac{\pi k}{L}\right)^2 D; \quad k = 0, 1, \dots \quad (6.10)$$

and that for each k , the sets of functions

$$e_0 = \frac{1}{\sqrt{(2L)}} \quad -L < x < L; \quad (6.11)$$

$$e_k = \frac{1}{\sqrt{L}} \cos\left(\frac{\pi k}{L}x\right) \quad -L < x < L; \quad k = 1, 2, \dots \quad (6.12)$$

$$o_k = \frac{1}{\sqrt{L}} \sin\left(\frac{\pi k}{L}x\right) \quad -L < x < L; \quad k = 1, 2, \dots \quad (6.13)$$

are orthonormal sets of even and odd eigenfunctions of Eq. (6.5), all with period $2L$. Show that e_k and o_k have the same eigenvalue λ_k .

5. Consider Eq. (6.5) with the initial condition

$$n(x, 0) = f(x). \quad (6.14)$$

Show that, if f has a definite parity (even or odd), the solution of the PDE at all later time has the same parity. Conclude that the solution of the PDE can be expanded in a cosine respectively sine series when the initial condition is even or odd. (Even and odd half range expansions. See Kreyszig page 490).

6. Use this result to find the solution of Eq.(6.5) with absorbing, respectively reflecting boundary conditions in the half interval $(0, L)$ from the solution $n(x, t)$ in the extended interval $(-L, L)$ with periodic boundary conditions. The procedure is called *the method of images*.

Chapter 7

Fourier transform & data analysis

Target

In our fifth session, we learn how Fourier analysis can be used as a tool for data analysis. Hitherto we have considered functions of a 'space' variable. In this Section it is more natural to think of functions of time. Sampling such a function at a discrete points of time yields a time series.

Time series

Measurements produce time series of data points y_1, y_2, \dots, y_M , which describe the values of a time dependent physical quantity $y(t)$. If the measurements are taken every δt seconds, and the first measurement is taken at $t = \delta t$, y_j simply equals $y(j\delta t)$. From the data, one would like to draw conclusions on the properties of $y(t)$. The road from empirical data to theoretical inferences is strewn with pitfalls. Fourier series (and more generally Fourier transforms) can sometimes help along the way.

Even though measurements of $y(t)$ invariably produce discrete time series, we can assume for convenience that the sampling interval δt is so short that the time dependence of $y(t)$ is known with sufficient accuracy for a certain time interval $0 < t < T$. Furthermore, we assume that T is much larger than any physical time scale of the problem. E.g. if the function considered is periodic, T exceeds the period of the oscillation, and if parts of the signal decay exponentially, they must be nearly zero at $t = T$.

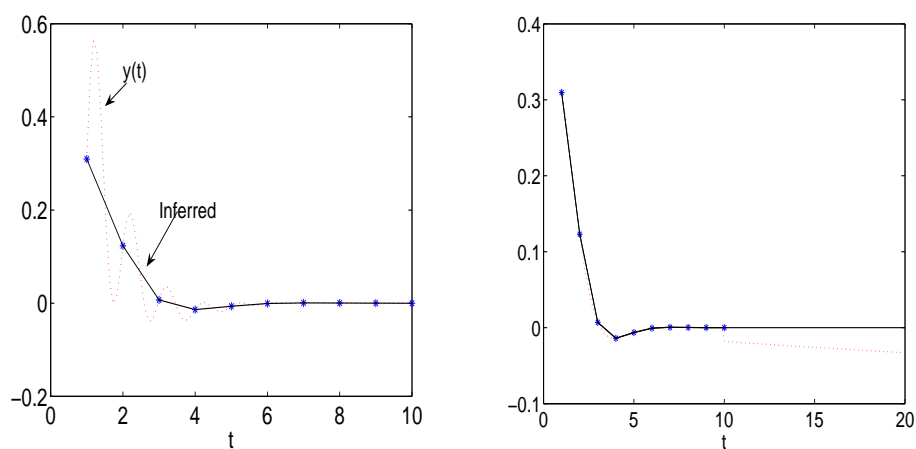


Figure 7.1: The left panel illustrates how a linear interpolation (black line) between known values (*) of a function (red dotted line) does not capture oscillations with a period shorter than δt . We do not know what really happens 'between' data points! The right panel illustrates that inferences beyond the observation range can easily be off the mark. These points are obvious, yet often neglected.

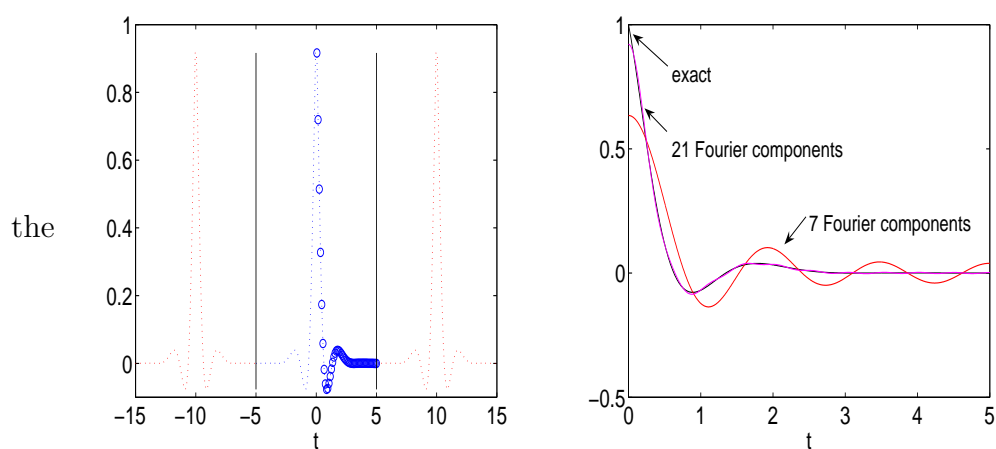


Figure 7.2: Left panel: The ‘measured’ $y(t)$ values in the interval $0 < t < T$, with $T = 5$ are indicated by blue circles. The function y is symmetrically extended to the interval $-T < t < T$ (blue dotted line). The red dotted line is the periodic function obtained by inverting the Fourier series for y . Right panel: including a finite number of Fourier components (7 and 21) provides approximation of different quality to the function y .

To apply Fourier analysis, we *conceptually* extend our data to the interval $-T < t < T$, which is symmetric around zero. ("Conceptually" means that we do not actually tamper with the data). We extend the range using the definition:

$$y(t) = y(-t); \quad -T < -t < 0. \quad (7.1)$$

Due to symmetry, the Fourier coefficient for the extended function are all real and given by the cosine Fourier series. Denoting, as usual, the k 'th Fourier coefficients by \hat{y}_k , the function is represented by the Fourier series

$$y_F(t) = \hat{y}_0 + \lim_{M \rightarrow \infty} \sum_{n=1}^M \hat{y}_n \cos\left(\frac{\pi n t}{T}\right), \quad (7.2)$$

where

$$\hat{y}_0 = \frac{1}{T} \int_0^T y(t) dt \quad (7.3)$$

$$\hat{y}_n = \frac{2}{T} \int_0^T \cos\left(\frac{\pi n t}{T}\right) y(t) dt \quad \text{for } n > 1. \quad (7.4)$$

Conforming to standard usage, we adopt a slightly different normalization convention: the factor $1/\sqrt{M}$ is omitted from the inverse Fourier transform and is replaced by $1/M$ in the definition of the Fourier coefficients.

1. We would like to believe that $y_F = y$, but how should we interpret the equality sign? In what sense y_F is 'the same' function as y is an issue well described in the mathematical literature. Find out more, and illustrate your findings with relevant plots.
2. The function $y(t)$ used in the examples is

$$y(t) = \exp(-2t)(\sin(t/2) + \cos(3t)), \quad 0 < t < 5. \quad (7.5)$$

Explain why the approximate Fourier representation with 21 modes does relatively poorly near $x = 0$, see Fig.(7.2).

3. In principle, one could choose an odd extension of the function y and describe the same problem with a sine half-range series. Why is it preferable to use an even extension?

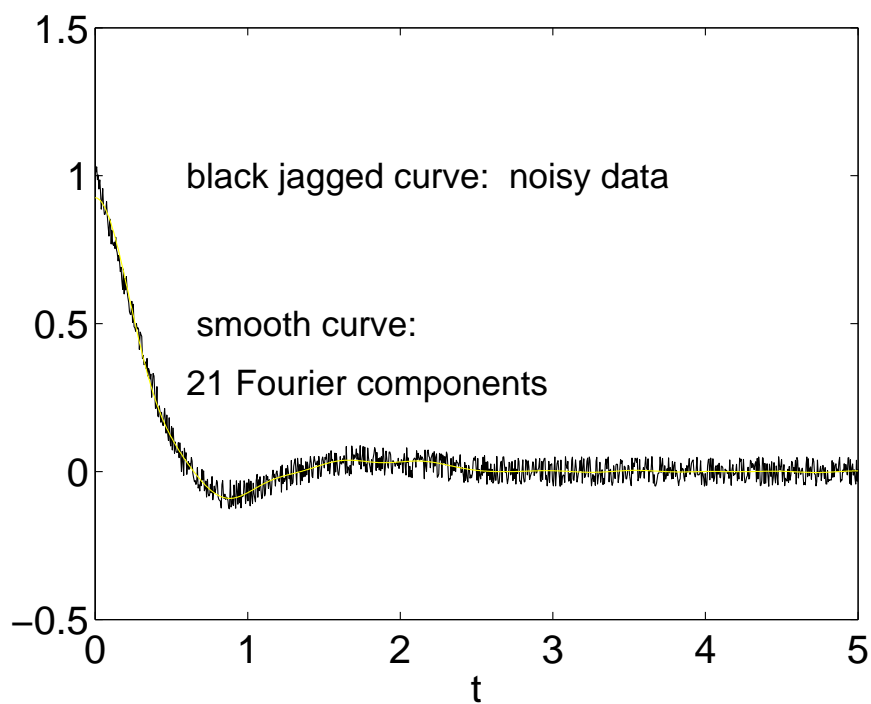


Figure 7.3: The ‘measured’ $y(t)$ is affected by high frequency random noise: each measured value comprises the ‘true’ value (whatever that is), plus a random number drawn from a uniform distribution. Random numbers belonging to different data points are statistically independent. The noisy character of the data gives $y(t)$ its irregular jagged shape. The smooth yellow line is obtained using a Fourier transform with a high frequency cut-off

4. A Fourier transform can be used to filter (remove) noise from data. Perturb a function y of your own choice with a small amount of additive noise, i.e. add at each point a small random number. Fourier transform, remove the high frequency components, and inverse Fourier transform. How does the result compare with the unperturbed data?
5. Try and explain your findings with theoretical arguments.

Chapter 8

Small oscillations & the wave equation

Target

In our fourth session, we learn about normal modes, and how small oscillations propagate in elastically coupled systems.

Elastically coupled systems

In many physical applications, n particles with space positions r_1, r_2, \dots, r_n interact via a potential $V(r_1, r_2, \dots, r_n)$. E.g., in solids, atoms or molecules can oscillate around fixed 'equilibrium' positions $r_1^e, r_2^e, \dots, r_n^e$. These equilibrium positions are all stationary points of the potential interaction energy. For small oscillations the potential energy of a displacement around a stationary state can be approximated by a quadratic function of the coordinates.

To be specific, let us consider M particles of equal mass m , which are placed on a linear grid and can move in a direction perpendicular to the grid. The time dependent displacement vector of the full system is denoted by \mathbf{y} . The displacement of particle j is the j 'th coordinate of \mathbf{y} . We assume periodic boundary conditions, meaning that the points $j = 0$ and $j = m$ are considered identical, or equivalently, that the particles are placed on a ring.

1. Argue that the interaction energy can be written as

$$V(\mathbf{y}) = \frac{\kappa}{2} \sum_{j=1}^M (y_j - y_{j-1})^2. \quad (8.1)$$

2. Consider a vector \mathbf{f} whose j 'th coordinate is the force on the j 'th particle. Show that the force vector corresponding to V has the form

$$\mathbf{f} = \kappa \Delta^2 \mathbf{y}. \quad (8.2)$$

3. Using Newton's II law, show that

$$\frac{d^2 \mathbf{y}}{dt^2} = \frac{\kappa}{m} \Delta^2 \mathbf{y}. \quad (8.3)$$

4. Using a Fourier series representation

$$\mathbf{y}(t) = \sum_{k=0}^{M-1} \hat{y}_k(t) \mathbf{F}_k, \quad (8.4)$$

show that the time dependent Fourier coefficients $\hat{y}_k(t)$ obey the equations

$$\frac{d^2 \hat{y}_k(t)}{dt^2} = \omega_0^2 \lambda_k \hat{y}_k(t), \quad k = 0, 1, \dots, M-1, \quad (8.5)$$

where λ_k are the previously discussed eigenvalues of the discrete Laplacian and where $\omega_0^2 = \frac{\kappa}{m}$.

5. Solve the equation of motion with the following initial conditions:

- (a) $\mathbf{y}(t=0) = \mathbf{F}_1$ and $\frac{d\mathbf{y}(t=0)}{dt} = 0$
 (b) $y(j, t=0) = \delta_{j5}$ and $\frac{dy(j, t=0)}{dt} = 0$.

6. Discuss differences and similarities with the diffusion equation.
 7. Show that the interaction energy of a configuration \mathbf{y} can be written in terms of its Fourier coefficients as

$$V(\mathbf{y}) = \frac{\kappa}{2} \sum_{k=0}^{M-1} |\lambda_k| |\hat{y}_k|^2. \quad (8.6)$$

Hint: Let $S\mathbf{y}$ denote the right shifted vector with coordinates y_{j-1} . From Eq. (8.1) we see that $V = \kappa/2 \|\mathbf{y} - S\mathbf{y}\|^2$. We can now use that the Fourier transform is an isometry.

8. Show that the total energy can be written as

$$H(\mathbf{y}) = \frac{m}{2} \sum_{k=0}^{M-1} \left| \frac{d\hat{y}_k}{dt} \right|^2 + \frac{\kappa}{2} \sum_{k=0}^{M-1} |\lambda_k| |\hat{y}_k|^2 \quad (8.7)$$

In the Fourier basis the energy appears as a sum of contributions from independent modes. These are the normal modes of the problem.