Lecture Notes for Phys 780 "Mathematical Physics"

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Abstract

These lecture notes will contain some additional material related to Arfken & Weber, 6th ed. (*abbreviated* **Arfken**), which is the main textbook. Notes for all lectures will be kept in a single file and the table of contents will be automatically updated so that each time you can print out only the updated part.

Please report any typos to vitaly@oak.njit.edu

Contents

I Introduction

Foreword

These notes will provide a description of topics which are not covered in **Arfken** in order to keep the course self-contained. Topics fully explained in **Arfken** will be described more briefly and in such cases sections from **Arfken** which require an in-depth analysis will be indicated as **work-through: ...** . Occasionally you will have reading assignments - indicated as *READING: ...* . (Do not expect to understand everything in such cases, but it is always useful to see a more general picture, even if a bit faint.)

Homeworks are important part of the course; they are indicated as **HW***: ...* and include both problems from **Arfken** and unfinished proofs/verifications from notes. The HW solutions must be clearly written in pen (black or blue).

Part I

Introduction

I. VECTORS AND VECTOR CALCULUS

A. Vectors

A *vector* is characterized by the following *three* properties:

- has a magnitude
- has direction (Equivalently, has several components in a selected system of coordinates).
- obeys certain addition rules ("rule of parallelogram"). (Equivalently, components of a vector are transformed according to certain rules if the system of coordinates is rotated).

This is in contrast to a *scalar*, which has only magnitude and which is *not* changed when a system of coordinates is rotated.

How do we know which physical quantity is a vector, which is a scalar and which is neither? From experiment (of course). More general objects are *tensors* of higher rank, which transform in more compicated way. Vector is tensor of a first rank and scalr - tensor of zero rank. Just as vector is represented by a row (column) of numbers, tensor of 2d rank is represented by a matrix. (although matrices also appear indifferent contexes, e.g. for systems of linear equations).

1. Single vector

Consider a vector $\vec{a}$ with components a_x and a_y (let's talk 2D for a while). There is an associated scalar, namely the magnitude (or length) given by the Pythagoras theorem

$$a \equiv |\vec{a}| = \sqrt{a_x^2 + a_y^2} \tag{1}$$

Note that for a different system of coordinates with axes x', y' the components $a_{x'}$ and $a_{y'}$ can be very different, but the length in eq. (1) , obviously, will not change, which just means that it is a scalar.

Another operation allowed on a single vector is multiplication by a scalar. Note that the physical dimension ("units") of the resulting vector can be different from the original, as in $\vec{F} = m\vec{a}$.

2. Two vectors: addition

For two vectors, $\vec{a}$ and $\vec{b}$ one can define their sum $\vec{c} = \vec{a} + \vec{b}$ with components

$$c_x = a_x + b_x \ , \quad c_y = a_y + b_y \tag{2}$$

The magnitude of $\vec{c}$ then follows from eq. (1). Note that physical dimensions of $\vec{a}$ and $\vec{b}$ must be identical.

3. Two vectors: scalar product

If $\vec{a}$ and $\vec{b}$ make an angle ϕ with each other, their scalar (dotted) product is defined as $\vec{a} \cdot \vec{b} = ab\cos(\phi)$, or in components

$$\vec{a} \cdot \vec{b} = a_x b_x + a_y b_y \tag{3}$$

A different system of coordinates can be used, with different individual components but with the same result. For two orthogonal vectors $\vec{a} \cdot \vec{b} = 0$. The main application of the scalar product is the concept of work $\Delta W = \vec{F} \cdot \Delta\vec{r}$, with $\Delta\vec{r}$ being the displacement. Force which is perpendicular to displacement does not work!

4. Two vectors: vector product

At this point we must proceed to the 3D space. Important here is the correct system of coordinates, as in Fig. 1. You can rotate the system of coordinates any way you like, but you cannot reflect it in a mirror (which would switch right and left hands). If $\vec{a}$ and $\vec{b}$ make an angle $\phi \leq 180^o$ with each other, their vector (cross) product $\vec{c} = \vec{a} \times \vec{b}$ has a magnitude

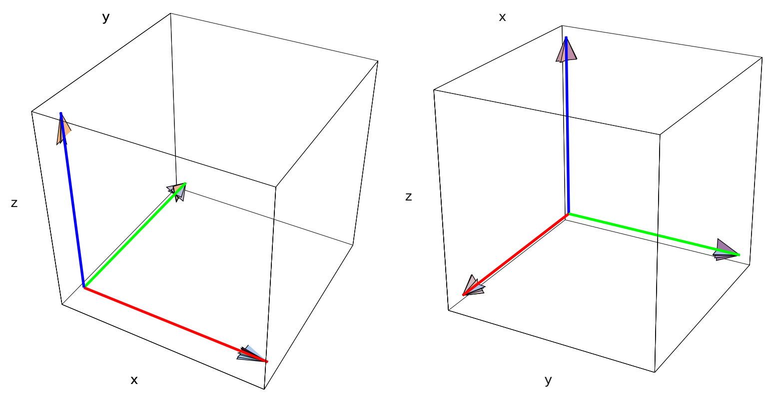

FIG. 1: The correct, "right-hand" systems of coordinates. Checkpoint - curl fingers of the RIGHT hand from x (red) to y (green), then the thumb should point into the z direction (blue). (Note that axes labeling of the figures is outside of the boxes, not necessarily near the corresponding axes.

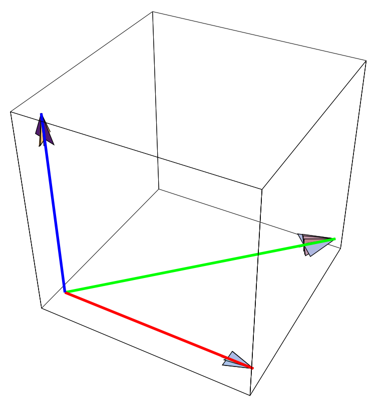

FIG. 2: Example of a cross product $\vec{c}$ (blue) $= \vec{a}$ (red) $\times\ \vec{b}$ (green). (If you have no colors, $\vec{c}$ is vertical in the example, $\vec{a}$ is along the front edge to lower right, $\vec{b}$ is diagonal).

$c = ab\sin(\phi)$. The direction is defined as perpendicular to both $\vec{a}$ and $\vec{b}$ using the following rule: curl the fingers of the right hand from $\vec{a}$ to $\vec{b}$ in the shortest direction (i.e., the angle must be smaller than 180^o). Then the thumb points in the $\vec{c}$ direction. Check with Fig. 2.

Changing the order changes the sign, $\vec{b} \times \vec{a} = -\vec{a} \times \vec{b}$. In particular, $\vec{a} \times \vec{a} = \vec{0}$. More generally, the cross product is zero for any two parallel vectors.

Suppose now a system of coordinates is introduced with unit vectors $\hat{i}$, $\hat{j}$ and $\hat{k}$ pointing in the x, y and z directions, respectively. First of all, if $\hat{i}$, $\hat{j}, \hat{k}$ are written "in a ring", the cross product of any two of them equals the third one in clockwise direction, i.e. $\hat{i} \times \hat{j} = \hat{k}$, $\hat{j} \times \hat{k} = \hat{i}$, etc. (check this for Fig. 1 !). More generally, the cross product is now expressed as a 3-by-3 determinant

$$\vec{a} \times \vec{b} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix} = \hat{i} \begin{vmatrix} a_y & a_z \\ b_y & b_z \end{vmatrix} - \hat{j} \begin{vmatrix} a_x & a_z \\ b_x & b_z \end{vmatrix} + \hat{k} \begin{vmatrix} a_x & a_y \\ b_x & b_y \end{vmatrix} \tag{4}$$

The two-by-two determinants can be easily expanded. In practice, there will be many zeroes, so calculations are not too hard.

B. Rotational matrix

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \tag{5}$$

HW: *Show that det* $[A_{rot}] = 1$

HW: *Show that rows are orthogonal to each other* **HW**: *write a "reflection matrix" which reflects with respect to the* y*-axes.*

In 3D rotation about the z-axis

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \hat{A}_z \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} , \ \hat{A}_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{6}$$

and similarly for the two other axes, with

$$\hat{A} = \hat{A}_x(\phi_1) \cdot \hat{A}_y(\phi_2) \cdot \hat{A}_z(\phi_3) \tag{7}$$

(order matters!)

C. Notations and summation convention

Components of a vector in selected coordinates are indicated by Greek or Roman indexes and summation of repeated indexes from 1 to 3 is implied, e.g.

$$a^2 = \vec{a} \cdot \vec{a} = \sum_{\alpha=1}^{3} a_\alpha a_\alpha = a_\alpha a_\alpha \tag{8}$$

(summation over other indexes, which are unrelated to components of a vector, will be indicated explicitly). Lower and upper indexes are equivalent at this stage. The notation

x^α will correspond to $x\,,y\,,z$ with $\alpha = 1\,2\,3$, respectively and r^α will be used in the same sense.

Scalar product:

$$\vec{a} \cdot \vec{b} = a_\alpha b_\alpha$$

Change of components upon rotation of coordinates

$$a'_\alpha = A_{\alpha\beta} a_\beta \tag{9}$$

The Kronecker delta symbol $\delta^{\alpha\beta}$ will be used, e.g.

$$a^2 = a^\alpha a^\beta \delta^{\alpha\beta}\,,\ \vec{a} \cdot \vec{b} = a_\alpha b_\beta \delta_{\alpha\beta} \tag{10}$$

(which is a second-rank *tensor*, while $\vec{a}$ is tensor of the 1st rank).

For terms involving vector product a full antisymmetric tensor $\epsilon_{\alpha\beta\gamma}$ ("Levi-Civita symbol") will be used. It is defined as $\epsilon_{1,2,3} = 1$ and so are all components which follow after an even permutation of indexes. Components which have an odd permutation, e.g. $\epsilon_{2,1,3}$ are -1 and all other are 0. Then

$$\left(\vec{a} \times \vec{b}\right)_\alpha = \epsilon_{\alpha\beta\gamma} a_\beta b_\gamma \tag{11}$$

Useful identities (not in **Arfken**):

$$\epsilon_{ikl}\epsilon_{mnl} = \delta_{im}\delta_{kn} - \delta_{in}\delta_{km} \tag{12}$$

$$\epsilon_{ikl}\epsilon_{mkl} = 2\delta_{im} \tag{13}$$

$$\epsilon_{ikl}\epsilon_{ikl} = 6 \tag{14}$$

HW: *Prove the above. Use*

$$\left(\vec{a} \times \vec{b}\right)^2 = a^2 b^2 - \left(\vec{a} \cdot \vec{b}\right)^2$$

for the 1st one and

$$\delta_{ii} = 3$$

for the other two.

HW: *Prove the 1st three identities from the inner cover of Jackson*

D. Derivatives

Operator $\hat{\nabla}$:

$$\hat{\nabla} = \vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z} \tag{15}$$

(Cartesian coordinates only!)

Then

$$\text{grad}\Phi \equiv \hat{\nabla}\Phi \equiv \frac{\partial}{\partial \vec{r}}\Phi \tag{16}$$

or in components

$$\left(\hat{\nabla}\Phi\right)_\alpha = \frac{\partial}{\partial x^\alpha}\Phi$$

Divergence:

$$\text{div}\vec{F} \equiv \hat{\nabla} \cdot \vec{F} = \frac{\partial}{\partial x^\alpha}F_\alpha \tag{17}$$

Curl:

$$\text{curl}\vec{F} \equiv \hat{\nabla} \times \vec{F} \tag{18}$$

or in components

$$\left(\text{curl}\vec{F}\right)_\alpha = \epsilon_{\alpha\beta\gamma}\frac{\partial}{\partial x^\beta}F_\gamma$$

HW: *Let* $\vec{r} = (x,\, y,\, z)$ *and* $r = |\vec{r}|$. *Find* $\hat{\nabla}r$, $\hat{\nabla} \cdot \vec{r}$, $\hat{\nabla} \times (\vec{\omega} \times \vec{r})$ *with* $\vec{\omega} = const$

Note gradΦ and curl$\vec{F}$ are genuine vectors, while div$\vec{F}$ is a true scalar.

Important relations:

$$\text{curl}\left(\text{grad}\Phi\right) = 0 \tag{19}$$

$$\text{div}\left(\text{curl}\vec{F}\right) = 0 \tag{20}$$

HW: *show the above*

HW: *(required) 1.3.3, 1.4.1,2,4,5,9,11*

1.5.3 (prove),4,6,7,10,12,13

1.6.1,3

1.7.5,6

1.8.3,10-14 1.9.2,3 (optional)

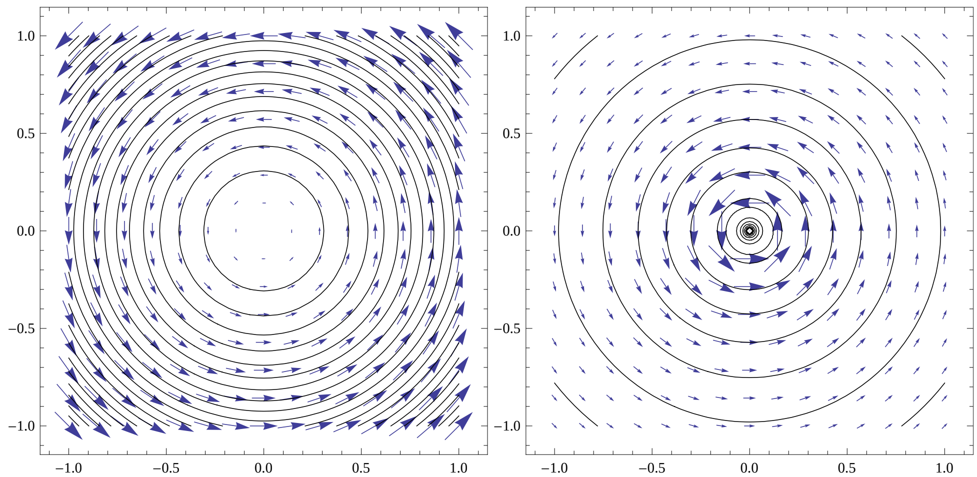

FIG. 3: Examples of fields with non-zero curl. Left - $\vec{\omega} \times \vec{r}$, velociity field of a rotating platform, similar to magnetic field *inside* a wire with current coming out of the page. Right - $\vec{\omega} \times \vec{r}/r^2$, similar (in 2D) to magnetic field *outside* an infinitely thin wire with current coming out of the page.

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E. Divergence theorem (Gauss)

$$\int\int\int_V \left(\hat{\nabla} \cdot \vec{F}\right) dV = \int\int_S \vec{F} \cdot \vec{n}\, da \tag{21}$$

Proof: first prove for an infinitesimal cube oriented along x, y, z; then extend for the full volume **HW**: *(optional) do that*

HW: *verify the Divergence theorem for $\vec{F} = \vec{r}$ and spherical volume*

HW: *1.11.1-4*

F. Stokes theorem

$$\int\int_S \left(\hat{\nabla} \times \vec{F}\right) \cdot \vec{n}\, da = \oint \vec{F} \cdot d\vec{l} \tag{22}$$

Proof: first prove for a plane ("Green's theorem") starting from an infinitesimal square; then generalize for arbitrary, non-planar surface

HW: *verify Stokes theorem for $\vec{F} = \omega \times \vec{r}$ and a circular shape.* **HW**: *1.12.1,2*

II. DIRAC DELTA

A. Basic definitons

$$\delta(x) = 0\ , \quad x \neq 0 \tag{23}$$
$$\delta(x) = \infty\ , \quad x = 0$$
$$\int_{-\epsilon}^{\epsilon} \delta(x)\, dx = 1\ , \quad \text{for any } \epsilon > 0$$

Then,

$$\int_{-\epsilon}^{\epsilon} \delta(x) f(x)\, dx = f(0)\ , \quad \text{for any } \epsilon > 0 \tag{24}$$

Note: the real meaning should be given only to integrals. E.g., $\delta(x)$ can oscillate infinitely fast, which does not contradict $\delta(x) = 0$ once an integral is taken.

Sequences leading to a δ-function for $n \to \infty$:

$$\delta_n(x) = n \text{ for } |x| < 1/2n\ , \quad 0 \text{ otherwise} \tag{25}$$

$$\delta_n(x) = \frac{n}{\pi} \frac{1}{n^2 x^2 + 1} \tag{26}$$
$$\delta_n(x) = \frac{n}{\sqrt{\pi}} \exp\left(-n^2 x^2\right) \tag{27}$$
$$\delta_n(x) = \frac{\sin(nx)}{\pi x} \tag{28}$$
$$\delta_n(x) = \frac{n}{2} \exp\left(-n|x|\right) \tag{29}$$

HW: *check normalization and reproduce plots*

Derivative:

$$\int \delta'(x) f(x) = -f'(0) \tag{30}$$

HW: *Show the above by integrating by parts; verify explicitly by using eq.(25); note that for finite n derivative of eq.(25) leads to $\pm\delta$*

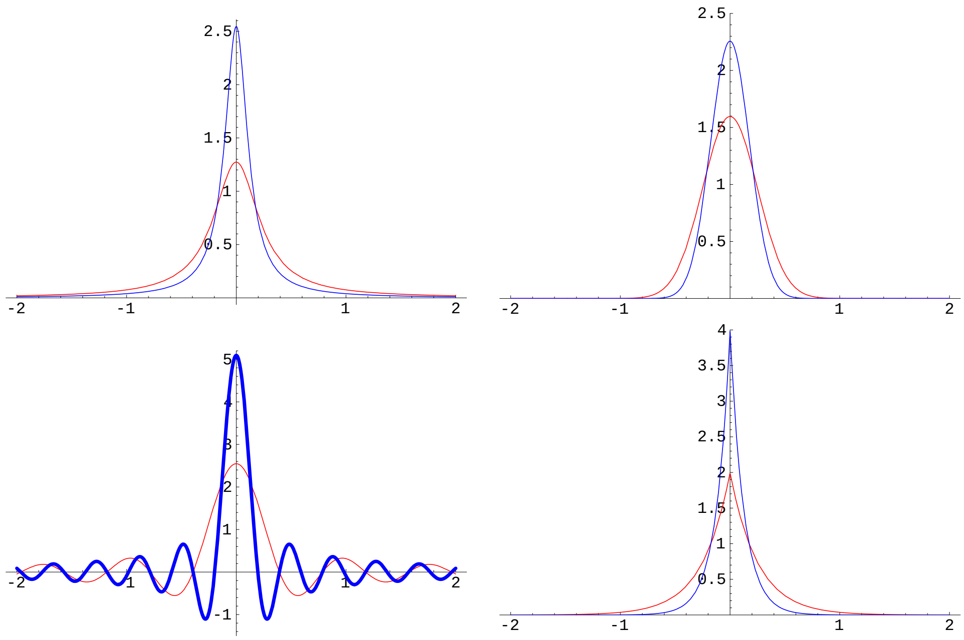

FIG. 4: Various represenations of δ_n which lead to Dirac delta-function for $n \to \infty$ - see eqs.(26-29).

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III. APPLICATIONS OF GAUSS THEOREM

A. Laplacian of $1/r$

$$\Delta\left(\frac{1}{r}\right) = -4\pi\delta\left(\vec{r}\right) \tag{31}$$

B. Integral definitions of differential operations

$$\hat{\nabla} \cdot \vec{a} = \lim_{V \to 0} \frac{1}{V} \oiint \vec{a} \cdot d\vec{S} \tag{32}$$

$$\hat{\nabla}\phi = \lim_{V \to 0} \frac{1}{V} \oiint \phi d\vec{S} \tag{33}$$

C. Green's theorems

$$\iiint dV \left(u\hat{\Delta}v - v\hat{\Delta}u\right) = \oiint d\vec{S} \cdot \left(u\hat{\nabla}v - v\hat{\nabla}u\right) \tag{34}$$

$$\iiint dV \left(u\hat{\Delta}v + \hat{\nabla}u \cdot \hat{\nabla}v\right) = \oiint d\vec{S} \cdot \left(u\hat{\nabla}v\right) \tag{35}$$

D. Vector field lines

(not in **Arfken**)

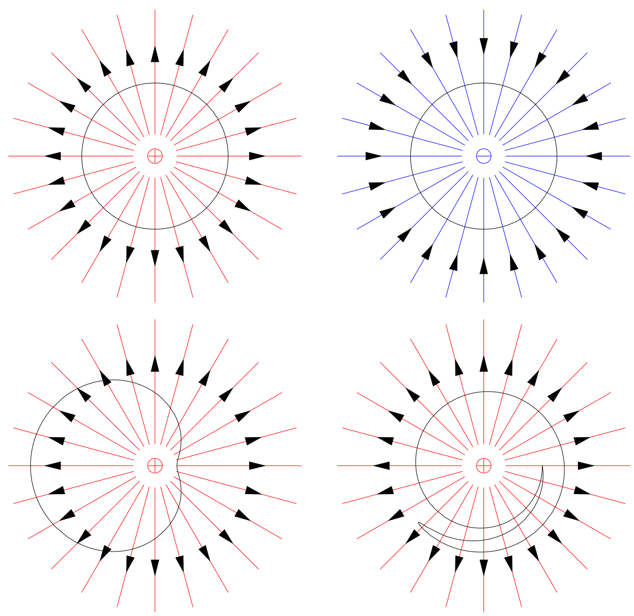

FIG. 5: Geometric meaning of Gauss theorem. The number of lines (positive or negative) is the flux. Lines are "conserved" in the domains with zero divergence.

IV. EXACT DIFFERENTIALS

V. MULTIDIMENSIONAL INTEGRATION

A. Change of variables

$$\int\int_R f(x,y)\,dx\,dy = \int\int_{R^*} f\left[x(u,v)\,,y(u,v)\right]\left|\partial(x,y)/\partial(u,v)\right|\;dudv \tag{36}$$

Here $|\partial(x,y)/\partial(u,v)|$ is the Jacobian. The 3D case is similar.

Cylindrical: (r,ϕ,z) with

$$x = r\cos\phi\;,\quad y = r\sin\phi \tag{37}$$

$$J = |\partial(x,y,z)/\partial(r,\phi,z)| = |\partial(x,y)/\partial(r,\phi)| = r$$

HW: *show the above*

Spherical: (r,θ,ϕ) with

$$x = r\sin\theta\cos\phi\;,\;\; y = r\sin\theta\sin\phi\;,\;\; z = r\cos\theta\;, \tag{38}$$

$$J = -r^2\sin\theta \tag{39}$$

HW: *show the above*

Solid angle:

$$d\Omega \equiv \frac{dA}{r^2} = \frac{1}{r^2}\frac{dV}{dr} = \sin\theta\,d\theta\,d\phi \tag{40}$$

$$\int d\Omega = 4\pi$$

HW: *show the above*

B. Multidimensional δ-function

$$\delta\left(\vec{r}-\vec{r}_0\right) = \delta\left(x-x_0\right)\delta\left(y-y_0\right)\delta\left(z-z_0\right) \tag{41}$$

$$\delta\left(u,v,w\right) = \left|\frac{\partial(x,y,z)}{\partial(u,v,w)}\right|\delta\left(x-x_0\right)\delta\left(y-y_0\right)\delta\left(z-z_0\right) \tag{42}$$

the rest will be discussed in class.

VI. CURVED COORDINATES

A. Metric tensor

$$dl^2 = g_{ik} dq_i dq_k = d\vec{q} \cdot \hat{g} \cdot d\vec{q} \tag{43}$$

Orthogonal coordinates:

$$g_{ik} = h_i^2 \delta_{ik} \text{ (no summation)} \tag{44}$$

HW: *Prove Green's theorems.*

1.10.1,2,5.

1.13.1,4,8,9

2.1.2,5

2.4.9, 2.5.9,18,19.

Get g_{ik} explicitly for polar coordinates.

VII. MATRICES

A. Geometric meaning of linear systems of equations

in class

B. Vector space and Gram-Schmidt ortogonalisation

in class

HW: *3.1.1-3,6*

C. Rectangular matrices, product

Examples of matrices, vector-rows and vector columns. Index-free notations. Innner and outer product. Transposition. Special matrices (identity, diagonal, symmetric, skew-symmetric, triangular).

D. Rank of a matrix

Definition. Equivalence of row and column rank.
Vector space: *if* $\vec{a}$ *and* $\vec{b}$ *part of v.s., then* $\alpha\vec{a} + \beta\vec{b}$ *also....* Dimension, basis.

1. *Rank and linear systems of equations (not in* **Arfken** *)*

Submatrix and augmented matrix.

$dim(A) = m \times n$, $dim\left(\vec{x}\right) = n$

$$\hat{A} \cdot \vec{x} = \vec{b} \tag{45}$$

a) existence: if $rank(A) = rank\left(\tilde{A}\right)$, $\tilde{A} \equiv \left(A|\vec{b}\right)$
b) uniqueness: if $rank(A) = rank\left(\tilde{A}\right) = n$

c) if $rank(A) = rank\left(\tilde{A}\right) = r < n$ - infinitely many solutions. Values of $n - r$ variables can be chosen arbitrary.

Homogeneous system:

$$\hat{A} \cdot \vec{x} = \vec{0} \tag{46}$$

a) alvays has a trivial solution $\vec{x} = \vec{0}$

b) if $rank(A) = n$ this solution is unique

c) if $rank(A) = r < n$ non-trivial solutions exist which form a vector space -*null* space- (together with $\vec{x} = \vec{0}$) with $dim = n - r$.

For $m < n$ (fewer equations than unknowns) - always non-trivial solution.

E. Formal operations with matrices:

$$A = B$$

$$\alpha A\,,\ \det(\alpha A) = \alpha^n \det A$$

AB can be zero

$$[A, B]$$

Jacobi identity. Commutation with diagonal matrix (the other must be diagonal too!)

F. Determinants

Explicit calculations. Operations with columns. Minor.

Square $n \times n$ matrix:

$$rank(A) < n \iff det(A) = 0 \tag{47}$$

Applications to linear equations. Cramer's rule: $x_1 = D_1/D, \ldots$.

Other properties:

$$\det A = \det A^T$$

$$\det(A.B) = \det(B.A) = \det(A)\det(B) \tag{48}$$

G. Inverse of a matrix

$$\det(A) \neq 0$$

$$\left(A^{-1}\right)_{jk} = \frac{1}{\det(A)}(-1)^{j+k} M_{kj} \tag{49}$$

(note different order!)

$$(AB)^{-1} = B^{-1}A^{-1} \tag{50}$$

HW: *find inverse of a* 2×2 *matrix with elements* a, b, c, d.

H. Trace

$$tr(A) \equiv A_{ii}\,,\ tr(A - B) = tr(A) - tr(B) \tag{51}$$

$$tr(AB) = tr(BA) \tag{52}$$

HW: *3.2.6(a),7,9*,10-13,20,23*,24,26,28,29,33*

I. Similarity transformations (real)

Let "operator" A

$$\vec{r}_1 = A \cdot \vec{r}$$

while B changes coordinates

$$B \cdot \vec{r} = \vec{r}'$$

Look for new A' so that

$$\vec{r}_1' = A' \cdot \vec{r}'$$

Then

$$A' = BAB^{-1} \tag{53}$$

If B orthogonal

$$A' = BAB^T \tag{54}$$

HW: *3.3.1,2,8,9*,10,12-14*,16*

J. Complex generalization

$$A^\dagger \equiv (A^*)^T$$

$H^\dagger = H$ -Hermitian

$U^\dagger = U^{-1}$ - unitary

$$(AB)^\dagger = B^\dagger A^\dagger \tag{55}$$

$$\langle\vec{a}|\vec{b}\rangle = a_i^* b_i\ ,\quad ||\vec{a}|| = \sqrt{\langle\vec{a}|\vec{a}\rangle} \tag{56}$$

Hermitian:

$$\langle a|H|b\rangle = \langle b|H|a\rangle^* \tag{57}$$

Unitary transsformation

$$A' = UAU^\dagger \tag{58}$$

HW: *reproduce eqs. 3.112-115*

3.4.1,3-8,12,14,26(a)*

K. The eigenvalue problem

$$\hat{A}\cdot\vec{x} = \lambda\vec{x} \tag{59}$$

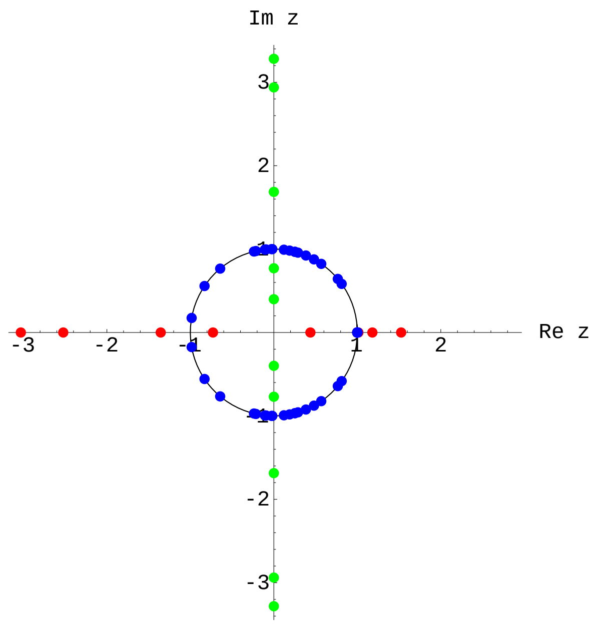

FIG. 6: Typical spectra of an orthogonal (blue), symmetric or Hermitian (red) and skew-symmetric (green) matrices.

$$\left(\hat{A} - \lambda \hat{I}\right) \cdot \vec{x} = \vec{0} \tag{60}$$

Thus,

$$det \left(\hat{A} - \lambda \hat{I}\right) = 0 \tag{61}$$

L. Spectrum

1. Hermitian: λ_i *- real*

proof in class

2. Unitary: $|\lambda_i| = 1$

proof in class

M. Eigenvectors

Eigenvectrors corresponding to distinct eigenvectors are orthogonal. This is true for both symmetric and orthogonal matrices. However, for orthogonal matrices the eigenvalues, and hence the eigenvectors will be complex. The definiton of the inner (dot) product then needs to be generalised:

$$\vec{a} \cdot \vec{b} = \sum_{i}^{N} \bar{a}_i b_i \tag{62}$$

where bar determines complex conjugation.

N. Similarity transformation

$$\tilde{A} = P^{-1} \cdot A \cdot P \tag{63}$$

with non-singular P.

Theorem 3 $\tilde{A}$ has the same eigenvalues as A and eigenvectors $P^{-1}\vec{x}$ where $\vec{x}$ is an eigenvector of A.

O. Diagonalization by similarity transformation

Let $\vec{x}_1, \vec{x}_2, \ldots \vec{x}_n$ be eigenvectors of an $n \times n$ matrix A with eigenvalues $\lambda_1, \ldots, \lambda_n$. Construct a matrix X with $\vec{x}_1, \vec{x}_2, \ldots \vec{x}_n$ as its columns. Then

$$D = X^{-1} \cdot A \cdot X = \mathrm{diag}\,[\lambda_1, \ldots, \lambda_n] \tag{64}$$

HW: *KR., p. 355, 1-3 (complete diagonalization); 4-6*

1. Specifics of symmetric matrices

If matrix A is symmetric, matrix X is orthonormal (or can be made such if normalised eigenvectors

$$\vec{e}_i = \frac{\vec{x}_i}{\sqrt{\vec{x}_i \cdot \vec{x}_i}}$$

are used). Then,

$$D = X^T \cdot A \cdot X \tag{65}$$

(orthogonal transformation) gives a diagonal matrix.

Major application: Quadratic forms

$$Q = \vec{x} \cdot A \cdot \vec{x} = \sum_{ij}^{n} x_i A_{ij} x_j \tag{66}$$

(a scalar!). With

$$y = X^T \cdot x \tag{67}$$

one gets

$$Q = \vec{y} \cdot D \cdot y = \lambda_1 y_1^2 + \ldots + \lambda_n y_n^2 \tag{68}$$

"Positively defined" - all $\lambda_i > 0$

Examples:

2. non-symmetric matrix via non-orthogonal similarity transformation

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

Matrix of eigenvectors (columns)

$$X = \begin{pmatrix} -i & i \\ 1 & 1 \end{pmatrix}$$

$$X^{-1} A X = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

3. Symmetric matrix via orthogonal transformation

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Eigenvectoros (columns, normalized):

$$O = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$O^T AO = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

4. Hermitian matrix via unitary transformation

$$A = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$U = \begin{pmatrix} \frac{i}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$U^\dagger AU = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

P. Spectral decomposition

$$H = \sum_i \lambda_i |e_i\rangle\langle e_i| \tag{69}$$

$$\hat{I} = \sum_i |e_i\rangle\langle e_i| \tag{70}$$

work-through: Examples 3.5.1,2

Q. Functions of matrices

$$e^A = \hat{I} + A + \frac{1}{2}AA + \dots$$

HW*: derive eq. 3.170a*

$$\det\left(e^{H}\right) = e^{tr(H)} \tag{71}$$

Spectral decomposition law:

$$f(H) = \sum_i f(\lambda_i)\, |e_i\rangle\langle e_i| \tag{72}$$

HW: *3.5.2,6,8*,10,16-18,30*

1. Exponential of a matrix: detailed example

Consider a matrix

$$\hat{A} = \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix}$$

- find eigenvalues

  With $\hat{I}$ being a 2×2 identity matrix

  $$\det\left(\hat{A} - \lambda \hat{I}\right) = 4 + \lambda^2 = 0$$

  thus

  $$\lambda_{1,2} = \pm 2i\,, \quad i = \sqrt{-1}$$

- find eigenvectors Let $\vec{a} = (x_1\,, x_2)$. Then $A \cdot \vec{a} = \lambda_{1,2}\vec{a}$ implies

  $$(2x_2\,,\ -2x_1) \ = \ \pm 2i\,(x_1\,,\ x_2)$$

  Thus

  $$x_2 = \pm i x_1$$

  or can select $x_2 = 1$, then

  $$\vec{a}_1 = (-i\,,\ 1)$$

  $$\vec{a}_2 = (+i\,,\ 1)$$

- construct a matrix X which would made $\hat{A}$ diagonal via the similarity transformation.

  Construct X as transpose of a matrix made of $\vec{a}_1\,,\ \vec{a}_2$:

  $$\hat{X} = \begin{pmatrix} -i & i \\ 1 & 1 \end{pmatrix}$$

with the inverse

$$\hat{X}^{-1} = \begin{pmatrix} i/2 & 1/2 \\ -i/2 & 1/2 \end{pmatrix}$$

Then

$$X^{-1} \cdot A \cdot X = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix}$$

as expected.

- Find $\exp\left(\hat{A}\right)$.

  Use an expansion

  $$\exp\left(\hat{A}\right) = \sum_{0}^{\infty} \frac{1}{n!} \hat{A}^n$$

  For every term

  $$A^n = A \cdot A \ldots A = XX^{-1}AXX^{-1}s \ldots XX^{-1}AXX^{-1}$$

  (since $XX^{-1} = I$). Introducing the diagonal

  $$\tilde{A} = X^{-1}AX$$

  one thus has

  $$A^n = X\tilde{A}^n X^{-1}$$

  and

  $$\exp(A) = X \exp\left(\tilde{A}\right) X^{-1} = X \begin{pmatrix} e^{\lambda_1} & 0 \\ 0 & e^{\lambda_2} \end{pmatrix} X^{-1} = \begin{pmatrix} \cos 2 & \sin 2 \\ -\sin 2 & \cos 2 \end{pmatrix}$$

R. Applications of matrix techniques to molecules

1. Rotation

(*Note: in this section $\hat{I}$ is rotational inertia tensor, not identity matrix*)

We will treat a molecule as a solid body with continuos distribution of mass described by density ρ. In terms of notations this is more convenient than summation over discrete atoms. Transition is given by a standard

$$\int \rho\left(\vec{r}\right) dV \left(\ldots\right) \rightarrow \sum_n m_n \left(\ldots\right) \tag{73}$$

with m_n being the mass of the n-th atom

For a solid body

$$\vec{v} = \vec{\Omega} \times \vec{r}$$

The kinetic energy is then

$$K = \frac{1}{2} \int \rho\left(\vec{r}\right) v^2 \left(\vec{r}\right) dV \tag{74}$$

With

$$\left(\vec{\Omega} \times \vec{r}\right)^2 = \Omega^2 r^2 - \left(\vec{\Omega} \cdot \vec{r}\right)^2$$

one gets

$$K = \frac{1}{2} \vec{\Omega} \cdot \hat{I} \cdot \vec{\Omega} \tag{75}$$

Here

$$I_{ik} = \int \rho \left(r^2 \delta_{ik} - r_i r_k\right) dV \tag{76}$$

is the rotational inertia tensor.

If the molecule is symmetric and axes are well chosen from the start, tensor I will be diagonal. Otherwise, one can make it diagonal by finding principal axes of rotation:

$$\hat{I} = \operatorname{diag}\left\{I_1\ ,\ I_2\ ,\ I_3\right\} \tag{77}$$

HW. Show that for a diatomic molecule with r being the separation between atoms

$$I = \mu r^2\ ,\ \ 1/\mu = 1/m_1 + 1/m_2 \tag{78}$$

with μ being the reduced mass.

2. *Vibrations of molecules*

We will need some information on mechanics.

Lagrange equation

$$\mathcal{L}\left(\vec{q},\ \dot{\vec{q}},\ t\right) = K - U \tag{79}$$

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} = \frac{\partial \mathcal{L}}{\partial q_i} \tag{80}$$

HW: *show that for a single particle with* $K = 1/2m\dot{x}^2$ *and* $U = U(x)$ *one gets the standard Newton's equation.*

Molecules

Let a set of 3D vectors $\vec{r}_n(t)$ $(n = 1, \ldots, N)$ determine the positions of atoms in a molecule, with r_n^0 being the equilibrium positions. We define a multidimensional vector

$$\vec{u}(t) = \left(\vec{r}_1 - \vec{r}_1^0\,,\ \ldots\ ,\vec{r}_N - \vec{r}_N^0\right) \tag{81}$$

With small deviations from equilibrium, both kinetic and potential energies are expected to be quadratic forms of $\dot{\vec{u}}$ and $\vec{u}$:

$$K = \frac{1}{2}\dot{\vec{u}} \cdot \hat{M} \cdot \dot{\vec{u}} > 0 \tag{82}$$

$$U = \frac{1}{2}\vec{u} \cdot \hat{k} \cdot \vec{u} \geq 0 \tag{83}$$

Introduce "inertial matrix"

$$\hat{M} = \frac{\partial}{\partial \dot{\vec{u}}}\frac{\partial}{\partial \dot{\vec{u}}}\mathcal{L} \tag{84}$$

and "elastic matrix"

$$\hat{k} = -\frac{\partial}{\partial \vec{u}}\frac{\partial}{\partial \vec{u}}\mathcal{L} \tag{85}$$

Then the Lagrange equations take the form:

$$\hat{M} \cdot \ddot{\vec{u}} = -\hat{k} \cdot \vec{u} \tag{86}$$

We look for a solution

$$\vec{u}(t) = \vec{u}_0 \exp{(i\omega t)} \tag{87}$$

$$-\omega^2 \hat{M} \cdot \vec{u}_0 + \hat{k} \cdot \vec{u}_0 = 0 \tag{88}$$

$$\hat{M}^{-1} \cdot \hat{k} \cdot \vec{u}_0 = \omega^2 \vec{u}_0 \tag{89}$$

ω^2 - eigenvalues of a matrix $\hat{M}^{-1} \cdot \hat{k}$ ("secular matrix").

Normal coordinates

Once the secular equation is solved, one can find $3N$ generalized coordinates Q_α which are linear combinations of all $3N$ initial coordinates, so that

$$\mathcal{L} = \frac{1}{2} \sum_\alpha \left(\dot{Q}_\alpha^2 - \omega_\alpha^2 Q^2 \right) \tag{90}$$

Q_α determine shapes of characteristic vibrations

Example: diatomic molecule

$$\mathcal{L} = \frac{1}{2} \left(m_1 \dot{x}_1^2 + m_2 \dot{x}_2^2 \right) - \frac{1}{2} k_1 \left(x_2 - x_1 \right)^2$$

$$x_2 = -\frac{m_1 x_1}{m_2} \;, \quad X = x_2 - x_1$$

Now

$$\mathcal{L} = \frac{1}{2} \mu \dot{X}^2 - \frac{1}{2} k_1 X^2$$

with

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \tag{91}$$

and

$$\omega = \sqrt{\frac{k_1}{\mu}}$$

Above is a human way to solve the problem - we eliminated the motion of center of mass from the start and then found the frequency. A more formal, matrix way is...(in class)

VIII. HILBERT SPACE

work-through: Ch. 10.4 in Arfken *READING: Ch. 10.2-4*

Note: at this stage, you can treat the "weight function" $w(x) \equiv 1$

A. Space of functions

in class

B. Linearity

in class

C. Inner product

$$\langle f|g\rangle = \int_a^b dx\, f^* g \tag{92}$$

$$||f||^2 = \int_a^b dx\, |f|^2 \tag{93}$$

Orthonormal basis $|e_i\rangle$

$$\langle e_i|e_j\rangle = \delta_{ij}$$

$$f_i = \langle e_i|f\rangle\ ,\ \ |f\rangle = \sum_i f_i|e_i\rangle \tag{94}$$

$$\sum_i |e_i\rangle\langle e_i| = \hat{I}\ \rightarrow\ \delta\,(x-y) \tag{95}$$

Parceval identity:

$$||f||^2 = \sum_i |f_i|^2 \tag{96}$$

D. Completeness

$$\lim_{n\to\infty}\int_a^b dx\,\left|f(x)-\sum_i^n f_i e_i(x)\right|^2=0 \tag{97}$$

E. Example: Space of polynomials

Non-orthogonal basis

$$1,\,x,\,x^2,\,\ldots$$

Gram-Schmidt orthogonalization (in class). Leads to Legendre polynomials.

F. Linear operators

$$\hat{L}\left(a|f\rangle+b|g\rangle\right)=a\hat{L}|f\rangle+b\hat{L}|g\rangle$$

$$L_{ik}=\langle e_i|L|e_k\rangle$$

1. Hermitian

$$\langle f|L|g\rangle=\langle g|L|f\rangle^*\,,\quad L_{ik}=L_{ki}^* \tag{98}$$

$$\int_a^b dx\,f^*(x)\left(\hat{L}g(x)\right)=\int_a^b dx\,g(x)\left(\hat{L}f(x)\right)^* \tag{99}$$

2. Operator d^2/dx^2 . Is it Hermitian?

(in class)

HW: *10.1.15-17*

10.2.2,3,7,13*,14**

10.3.2

10.4.1,5a,10,11*

work-through: Examples 10.1.3 , 10.3.1

IX. FOURIER

work-through: Arfken , Ch. 14

$$\int_{-\pi}^{\pi} dx\, 1 \cdot \cos(nx) = 2\pi\delta_{n\,0} \tag{100}$$

$$\int_{-\pi}^{\pi} dx\, 1 \cdot \sin(nx) = 0$$

For m, $n \neq 0$:

$$\int_{-\pi}^{\pi} dx\, \cos(nx)\cos(mx) = \pi\,\delta_{mn} \tag{101}$$

$$\int_{-\pi}^{\pi} dx\, \cos(nx)\sin(mx) = 0$$

$$\int_{-\pi}^{\pi} dx\, \sin(nx)\sin(mx) = \pi\,\delta_{mn}$$

HW: *show/check the above*

A. Fourier series and formulas for coefficients

$$f(x) = a_0 + \sum_{n=1}^{\infty} \left(a_n \cos(nx) + b_n \sin(nx)\right) \tag{102}$$

Coefficients:

$$a_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi} dx\, f(x) \tag{103}$$

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} dx\, f(x)\cos(nx) \tag{104}$$

$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} dx\, f(x)\sin(nx) \tag{105}$$

Note: even function: $b_n = 0$; odd function: $a_n = 0$.

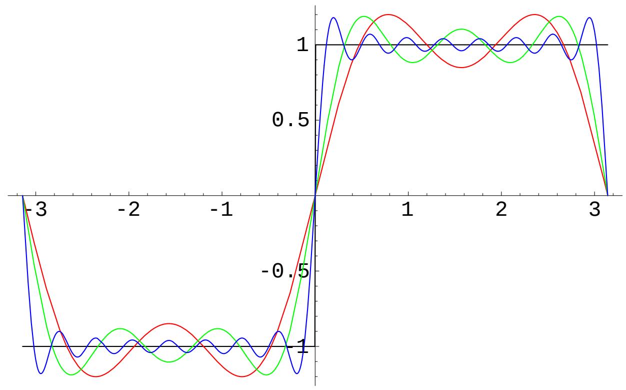

FIG. 7: Approximation of a square wave by finite numbers of Fourier terms (in class)

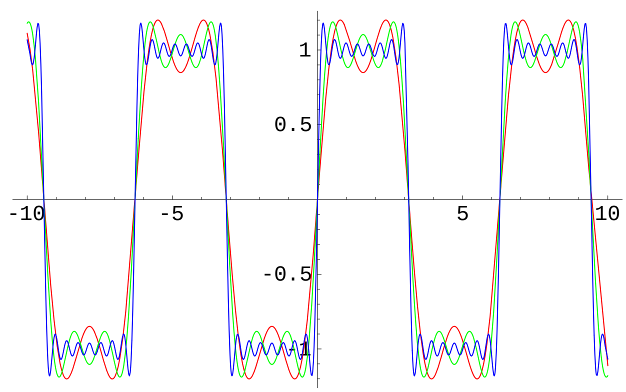

FIG. 8: Periodic extension of the original function by the Fourier approximation

B. Complex series

1. Orthogonality

"Scalar product" of two functions $f(x)$ and $g(x)$ on an interval $[-\pi, \pi]$:

$$\langle f|g\rangle = \int_{-\pi}^{\pi} dx\, f(x)^* g(x) \tag{106}$$

Introduce:

$$e_n(x) = e^{inx} \tag{107}$$

Then:

$$\langle e_n|\, e_m\rangle \equiv \int_{-\pi}^{\pi} dx\, e^{i(m-n)x} = 2\pi\delta_{mn} \tag{108}$$

(note: more compact than real sin/cos). **HW**: *Show/check that*

2. Series and coefficients

$$f(x) = \sum_{n=-\infty}^{n=\infty} c_n e^{inx} \tag{109}$$

or

$$|f\rangle = \sum_{n=-\infty}^{n=\infty} c_n \, |e_n\rangle \tag{110}$$

From orthogonality:

$$c_n = \frac{1}{2\pi} \langle e_n | \, f \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} dx \, e^{-inx} f(x) \tag{111}$$

Again, note much more compact than sin/cos.

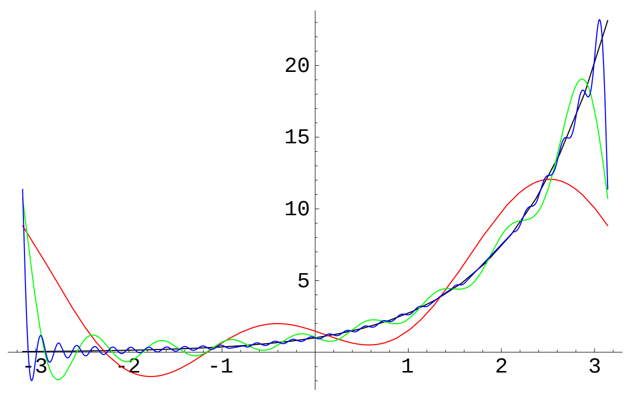

FIG. 9: Approximations of e^x by trigonometric polynomials (based on complex Fourier expansion). Red - 2-term, green - 8-term and blue - the 32 term approximations.

HW: *Expand* $\delta(x)$ *into* e^{inx}*.*

From **Arfken** *:*

14.1.3,5-7

14.2.3

14.3.1-4, 9a, 10a,b , 12-14

14.4.1,2a,3

C. Fourier vs Legendre expansions

(not in **Arfken**)

Consider the same square wave $f(x) = sign(x)\theta(1 - |x/\pi|)$ and an orthogonal basis

$$|p_n\rangle = P_n\left(\frac{x}{\pi}\right)$$

Then

$$|f\rangle = \sum_n c_n|p_n\rangle\ ,\ \ c_n = \langle p_n|f\rangle/||p_n||^2$$

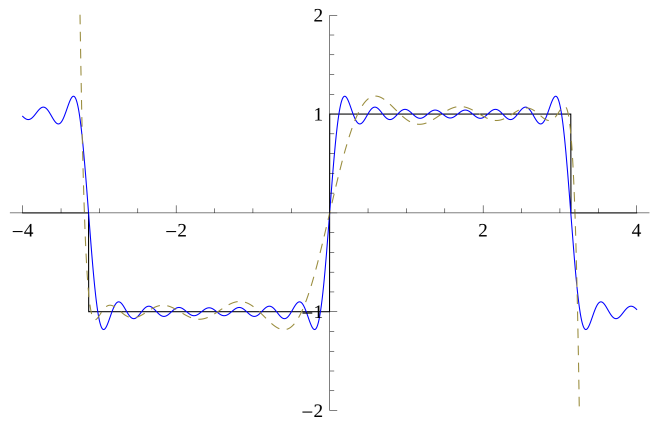

FIG. 10: Approximation of a square wave by $n = 16$ Fourier terms (blue) and Legendre terms (dashed)

X. FOURIER INTEGRAL

work-through: Ch. 15 (Fourier only). Examples: 15.1.1, 15.3.1

HW: *15.3.1-5,8,9,17a. 15.5.5*

A. General

in class

B. Power spectra for periodic and near-periodic functions

Note

$$\mathcal{F}\left[1\right] = \sqrt{2\pi}\delta\left(k\right) \tag{112}$$

Similarly,

$$\mathcal{F}\left[e^{-ik_0x}\right] = \sqrt{2\pi}\delta\left(k - k_0\right) \tag{113}$$

i.e. an ideally periodic signal gives an infinite peak in the power spectrum.

A real signal can lead to a finite peak for 2 major reasons:

- signal is not completely periodic
- the observation time is *finite*

This is illustrated in Fig. 12.

C. Convolution theorem

$$\mathcal{F}\left[\int_{-\infty}^{\infty} f(y)g(x-y)\,dy\right] = \sqrt{2\pi}\mathcal{F}\left[f\right]\mathcal{F}\left[g\right] \tag{114}$$

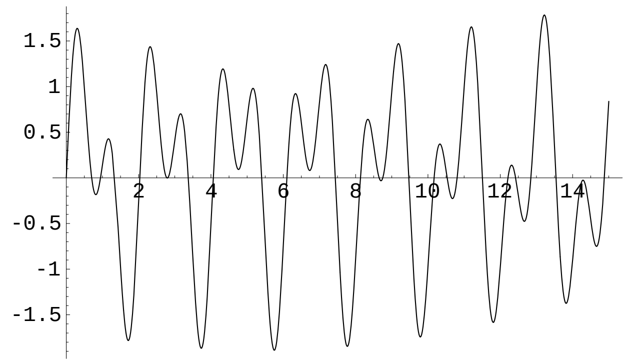

FIG. 11: An "almost periodic" function $e^{-0.001x}\left(\sin(3x)+0.9\sin(2\pi x)\right)$

D. Discrete Fourier

Consider various lists of N (complex) numbers. They can be treated as vectors, and any vector $\vec{f}$ can be expanded with respect to a basis:

$$\vec{f}=\sum_{n=1}^{N} f_n \vec{e}_n \tag{115}$$

with

$$\vec{e}_1=(1,0,0,\ldots)\ ,\ \vec{e}_2=(0,1,0,\ldots)\ ,\ \ldots \tag{116}$$

Scalar (inner) product is defined as

$$\vec{f}\cdot\vec{g}=\sum_{n=1}^{N} f_n^* g_n \tag{117}$$

(note complex conjugation).

Alternatively, one can use another basis with

$$\vec{e}_n{}'=\left(1,\, e^{2\pi i\,(2-1)\,(n-1)/N}\,,\ \ldots\,,\ e^{2\pi i\,(m-1)\,(n-1)/N}\,,\ \ldots\,,\ e^{2\pi i\,(N-1)\,(n-1)/N}\right) \tag{118}$$

Note: ssome books use m instead of our $(m-1)$ but their sum is then from 0 to $N-1$, so it is the same thing.

1. *Orthogonality*

$$\vec{e}_n{}'\cdot\vec{e}_k{}'=N\delta_{nk} \tag{119}$$

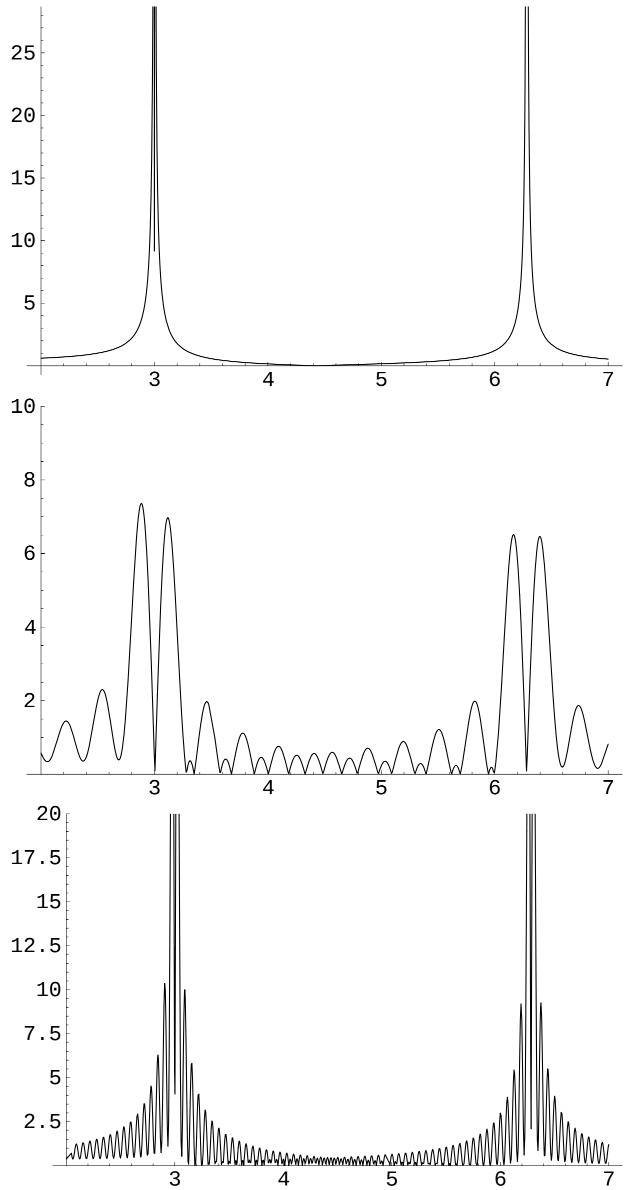

FIG. 12: Power spectrum of the previous function obtained using a cos Forier transformation (infinite interval) and finite intervals $L = 10$ and $L = 100$.

Indeed,

$$\vec{e}_n{}' \cdot \vec{e}_k{}' = \sum_{m=1}^{N} r^{(k-n)(m-1)} \; , \quad r \equiv e^{2\pi i/N} \tag{120}$$

Summation gives

$$\vec{e}_n{}' \cdot \vec{e}_k{}' = \frac{1 - r^{(k-n)N}}{1 - r^{(k-n)}} \tag{121}$$

Note that for k, n integer the numerator is always zero. The denominator is non-zero for any $k-n \neq 0$, which leads to a zero result. For $k=n$ one needs to take a limit $k \to n$

HW: *do the above*

Now we can construct a matrix ("Fourier matrix" $\hat{F}$) of $\vec{e}_n{}'$ for all $n \leq N$ and use it to get components in a new basis

$$\hat{F} \cdot \vec{f} \tag{122}$$

This will be Fourier transform. Applications will be discussed in class.

HW: *construct* $\hat{F}$ *for* $N=3$

XI. COMPLEX VARIABLES. I.

A. Basics: Permanence of algebraic form and Euler formula; DeMoivre formula; multivalued functions

in class

HW: *6.1.1-6,9,10,13-15,21*

B. Cauchy-Riemann conditions

$$f(z) = u(x,y) + iv(x,y)$$

If df/dz exists, then

$$u'_x = v'_y \ , \ u'_y = -v'_x \tag{123}$$

Also note:

$$\hat{\Delta}u = \hat{\Delta}v = 0 \tag{124}$$

and

$$\frac{u'_x}{u'_y}\frac{v'_x}{v'_y} = -1 \tag{125}$$

1. *Analytic and entire functions*

work-through: Examples 6.2.1,2

HW: *6.2.1a,2,8**

C. Cauchy integral theorem and formula

Any $f(z)$, analytic inside a simple C:

$$\oint_C f(z)dz = 0 \tag{126}$$

proof in class (from Stokes)

HW: *6.3.3*

$$f\left(z_0\right)=\frac{1}{2\pi i}\oint_C dz\,\frac{f(z)}{z-z_0} \tag{127}$$

$$f\left(z_0\right)^{(n)}=\frac{n!}{2\pi i}\oint_C dz\,\frac{f(z)}{\left(z-z_0\right)^{n+1}} \tag{128}$$

HW: *6.4.2,4,5,8a*

D. Taylor and Laurent expansions

in class

work-through: Ex. 6.5.1

HW: *6.5.1,2,5,6,8,10,11*

E. Singularities

in class

work-through: Ex. 6.6.1

HW: *6.6.1,2,5*

XII. COMPLEX VARIABLES. II. RESIDUES AND INTEGRATION.

HW: *7.1.1, 2a,b , 4,5,7-9,11,14,17,18*

in class

A. Saddle-point method

skip "theory" from **Arfken**

HW: *derive Stirling formula from*

$$\Gamma(n+1) = \int_0^\infty dx\, x^n e^{-x} \;, \;\; n \to \infty$$

Integral representation of Airy function:

$$Ai(x) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{z^3}{3} + zx\right) dz \tag{129}$$

Asymptotics:

$$Ai[x \gg 1] \sim \frac{1}{2\sqrt{\pi} x^{1/4}} \mathrm{e}^{-\frac{2}{3} x^{3/2}} \tag{130}$$

$$Ai[x \to -\infty] \sim \frac{1}{\sqrt{\pi}(-x)^{1/4}} \sin\left\{\frac{2}{3}(-x)^{3/2} + \frac{\pi}{4}\right\} \tag{131}$$

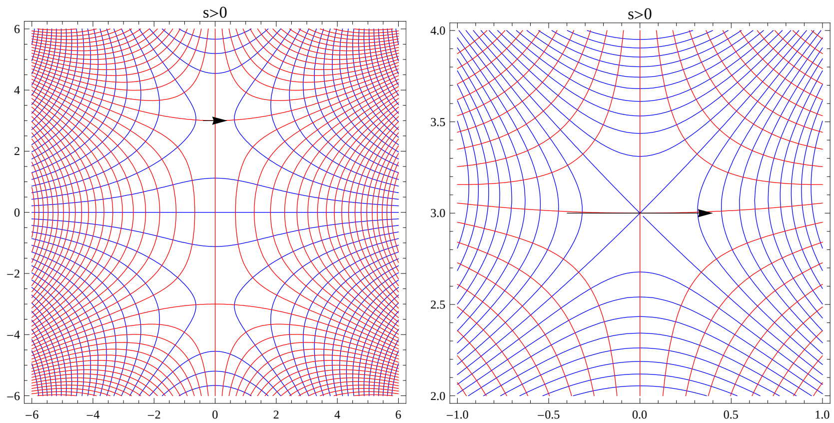

FIG. 13: The function $\phi(z)$ from the integrand e^{ϕ} of the Airy function $Ai(s)$ in the complex z-plane ($s = 9$). Blue lines - $Re[\phi] = const$, red lines - $Im[\phi] = const$. The saddles are at $z = \pm i\sqrt{s}$; arrow indicates direction of integration.

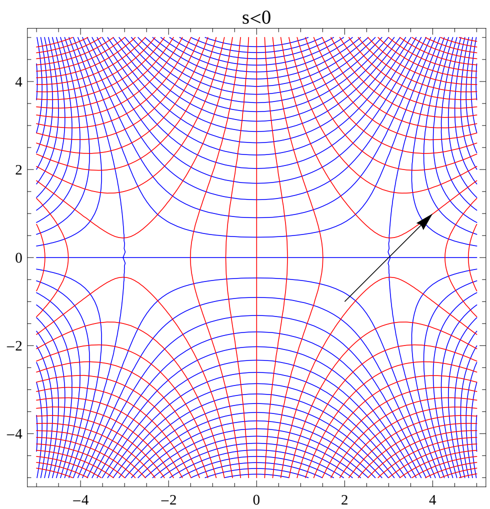

FIG. 14: Same, for $s = -9$.