Lecture Notes for Phys/MtSE 788 "Applied computational methods..."

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Abstract

We will first review the origin of the main special functions, their classification, physical origin and applications, and realization in Mathematica. It will take about 2-3 classes. The Mathematica files (with extension .m or .nb) will be given separately. *Note: do not get scared with all the math, since some of it is included for the purpose of completeness, and will not be discussed in class. This especially refers to non-numbered equations. During the class, you will be given more explicit instructions as to what can be skipped, and additional explanations also will be added.*

I will place a marker "=======" at the end of the latest update so you know where to terminate the printout for the coming class. Please do not print out notes for future lectures in advance since most of them will be updated.

Contents

Part I

Introduction

I. PHYSICS, ANALYTICS AND COMPUTATIONS

- Physics: very diverse scales; dimensionless parameter(s) $\rho_1\,,\,\rho_2\,,\ldots$ can span a huge domain from small to large values
- Analytics: dimensionless parameter(s) $\to\infty$ (or, $\to 0$)
- Computations: $\rho_1\,,\,\rho_2\,,\ldots\sim 1$
- Symbolic computations: more accurate analytics, less restrictions on parameters. Overlap with computations!

Example: Electrostatics. Distribution of fixed charges $q_1\,,q_2\,,\ldots$ located at $\vec{r}_1\,,\vec{r}_2\,,\ldots$. Origin of coordinates inside the domain. Need field (potential) everywhere.

- Physics: dimensionless parameter(s):

$$\rho\sim R/d\gg 1$$

R - distance from origin to the observation point. Or, for the observation point $\vec{r}$ close to charge No.1,

$$\rho_1=\left|\vec{r}-\vec{r}_1\right|/d\ll 1$$

- Analytics:

$$\phi\sim Q/R\;,\quad Q=q_1+q_2+\ldots\;,\quad R\gg d$$

$$\phi\sim q_1/\left|\vec{r}-\vec{r}_1\right|+const\;,\quad const=q_2/\left|\vec{r}_2-\vec{r}_1\right|+q_3/\left|\vec{r}_3-\vec{r}_1\right|+\ldots\;,\quad \left|\vec{r}-\vec{r}_1\right|\ll d$$

- Computations: can be done not too far from the system and not too close to charges (infinities!)

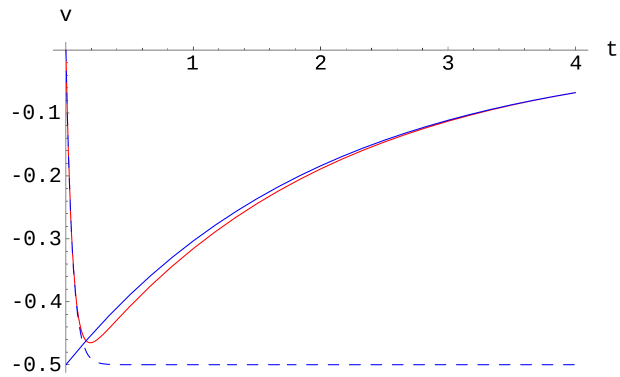

FIG. 1: Exact solution (red) and outer solution (blue) for $m = 0.1$. The blue dashed line is the "inner" solution - it is irrelevant for large times but accurately describes transient behavior for small $t \sim m$ (the "boundary layer"). Note that the large-t limit of the inner solution (horizontal dashed) and the small-t limit of the outer solution $-1/2$ are identical.

- Symbolic computations (*Mathematica*): systematic extension of the above expansions for a large number of terms (in terms of Legendre polynomials or in terms of multipoles - will not be discussed at the moment). Very useful if understand how many terms is needed.

- Graphics: needed for connection with physics. Small and large scales must be covered, and good graphics is possible if one understands the relation between them

II. AN OSCILLATOR WITH VANISHING MASS: IDEAS OF BOUNDARY LAYER AND SINGULAR PERTURBATIONS

Consider

$$m\ddot{x} + 2\dot{x} + x = 0 \tag{1}$$

with $x(0) = 1$, $\dot{x}(0) = 0$ and $m \to 0$. Could write

$$x = e^{-t/2}$$

but what about velocity?? - $\dot{x} = -(1/2)e^{-t/2}$ does not satisfy the initial condition. We can compare with exact solution and detect a "boundary layer" - see Fig. 1.

To understand velocity better, write an explicit equation

$$m\ddot{v} + 2\dot{v} + v = 0 \tag{2}$$

with $v(0)=0$, $m\dot{v}(0)=-1$ (from original equation). Neglect of m gives the "outer" solution

$$v^{out}=-\frac{1}{2}e^{-t/2} \tag{3}$$

which cannot satisfy both boundary conditions. To describe small times introduce a "stretched variable"

$$T=t/m^{\alpha}$$

and select α to have both terms with derivatives have the same order as $m\to 0$. This gives $\alpha=1$ and

$$\frac{d^2v}{dT^2}+2\frac{dv}{dT}=0 \tag{4}$$

which is an "inner" equation with solution

$$v^{in}(T)=e^{-2T}/2-1/2$$

Inner solution accurately describes the small times for a selected small (non-zero) m - see Fig. 1. Note that

$$v^{in}\left(T\to\infty\right)=v^{out}\left(t\to 0\right) \tag{5}$$

This is the basic principle of "matched asymptotic expansions".

Part II

Some special functions and their applications

III. INTRODUCTION

We know well elementary functions. sin, cos, *exp*. Where do special functions come from and what is their connection to elementary?

Consider

$$u''+I(x)u=0 \tag{6}$$

Now if $I(x) = const \equiv I$, one has for solutions $u(x)$

$$\sin\left(\sqrt{I}x\right)\ , \quad \cos\left(\sqrt{I}x\right)\ , \quad I > 0$$

$$\exp\left(\pm\sqrt{-I}x\right)\ , \quad I < 0$$

For $I(x) \neq const$ we have special functions.

Now what's qualitatively new (besides the special functions being harder to compute or sometimes even imagine)? New is the fact that $I(x)$ can change sign (!!!), leading to a transition from an oscillatory to exponential-type structure of the same solution in different domains of x. Already the simplest, Airy function described below has this property.

The other novelty is the possibility of $I(x_0) = \infty$ at some x_0 called a *singular point.* Now instead of the pair of independent solutions of type sin and cos which look extremely similar to each other, one will have two solutions with very different structure, depending on their behavior near x_0.

Near both types of points, zero and ∞ for $I(x)$, very interesting physics is expected. In this sense special functions are much more exciting than the elementary, which are somewhat dull in having the same behavior for all x (and an excursion into the complex plain will not make things much more exciting).

IV. GENERAL PROPERTIES OF THE SOLUTIONS

Since eq. (6) is a linear differential equation of the 2nd order, there are general properties which are equally applicable to sin, cos and to any of the special functions. For a specific non-elementary example, however, we will consider an equation

$$y'' - xy = 0 \tag{7}$$

which, leads to, in a sense the simplest non-elementary solutions - the Airy functions, see below.

A. Linear independence

First, there exist two linearly independent solutions, $\phi_1(x)$ and $\phi_2(x)$, which form a *fundamental* system of solutions. Any solution can be represented as

$$y(x) = C_1\phi_1(x) + C_2\phi_2(x) \tag{8}$$

with C_1, C_2 being arbitrary constants. Linear independence is tested by non-zero values of the *Wronskian*

$$W = \phi_1 \phi_2' - \phi_1' \phi_2 \neq 0 \tag{9}$$

In particular, if the original equation is already in the normal form (no 1st derivative), one has

$$W = const \tag{10}$$

HW: *Find Wronskian to the two Airy functions, and check eq.(10)[if you are good with Mathematica, write a pure function] .* **HW**: *(optional). Find an analog of eq. (10) for a full form of a general 2nd order equation. Hint: find dW/dx*

B. Oscillatory behavior

For $I(x) > 0$ in eq. (6), there will be oscillations in each of the fundamental solution see e.g., Fig. 2, similarly to sin and cos. Moreover, there exist a theorem that zeros of ϕ_1 and ϕ_2 alternate with each other, making the similarity even stronger. [In this context note that *both* ϕ_1, ϕ_2 oscillate, or both do not, as for $x > 0$ in Fig. 2)].

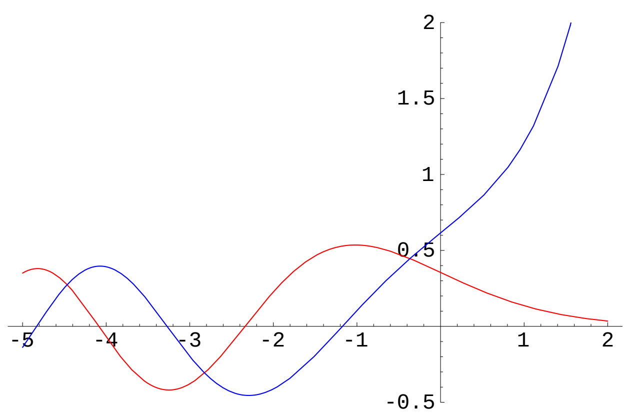

FIG. 2: Airy functions, Ai (red) and Bi (blue).

C. Singular points and classification of the solutions

If for $x \to x_0$, one has $I(x) \to \infty$, such a point x_0 is called *singular*. $x_0 = \infty$ is also a possibility (and this is the only singular point for the Airy equation above). There is a more fine classification based on how fast the ∞ is approached, but we will not use it now.

Remarkably, the solution does not always have to diverge at x_0. If $\phi(x_0)$ is finite, it is called the special function of the *first* kind. If it diverges, it is called of the *second* kind.

D. Asymptotics, and the WKB approximation

Let $I(x)$ in eq.(6) be large. Let us write it as $I(x) = -\rho^2 q(x)$ with $\rho \gg 1$ and make a substitution:

$$u(x) = \exp\left\{+\rho \int v(x)dx\right\}$$

which leads to

$$\rho v' + \rho^2 v^2 - \rho^2 q = 0 \tag{11}$$

HW: *(optional) show this* . Now solve by iterations:

$$v_0 = \pm\sqrt{q}$$

next

$$v_1 = -\frac{1}{\rho}\frac{v_0'}{2v_0}$$

Now

$$u(x) \propto \exp\left\{\rho\left[\pm\int\sqrt{q}dx\right] - 1/2\ln|\sqrt{q}|\right\}$$

or

$$u(x) \propto \frac{1}{|I|^{1/4}}\exp\left\{\pm\int\sqrt{-I(x)}dx\right\}$$

More explicitly, for $I(x) > 0$,

$$u(x) \propto \frac{1}{I^{1/4}}\sin\left\{\int I^{1/2}dx + \alpha\right\} \tag{12}$$

(α can have two values since 2 solutions), and for $I(x) < 0$

$$u(x) \propto \frac{1}{(-I)^{1/4}}\exp\left\{\pm\int(-I)^{1/2}dx\right\} \tag{13}$$

[small project (optional): write a Mathematica program for WKB (more than 2 iterations), apply to some known special function, and check the accuracy].

V. AIRY FUNCTIONS

Let us try to apply asymptotic analysis to Airy functions with $I(x) = -x$. It becomes large for $x \to \pm\infty$. One has

$$\int x^{1/2} dx = \frac{2}{3} x^{3/2}$$

which should be the argument in both the exponential and the oscillatory parts. This corresponds to the known asymptotics

$$Ai[x \gg 1] \sim \frac{1}{2\sqrt{\pi} x^{1/4}} \mathrm{e}^{-\frac{2}{3}x^{3/2}} \tag{14}$$

$$Ai[x \to -\infty] \sim \frac{1}{\sqrt{\pi}(-x)^{1/4}} \sin\left\{\frac{2}{3}(-x)^{3/2} + \frac{\pi}{4}\right\} \tag{15}$$

(and similarly for Bi "+" in the exp, and cos instead of sin). The exact proportionality factors come from the integral representation. The value of the constant in sin is selected to ensure transition to the decaying exponent on the other side of $x = 0$. [HW: plot asymptotes together with the Airy functions].

We know practically everything: the differential equation, the picture and the asymptotes. What can be added, is the integral representation and the physical problem where it appeared.

One has

$$Ai(x) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{z^3}{3} + zx\right) dz \tag{16}$$

As to physics, the above "rainbow integral" was introduced by Airy in the context of rainbow formation, beyond the geometrical optics. Recall that geometrical optics can predict the angle at which we see the rainbow via formation of a "caustic" - see Fig. 3, but it predicts an infinite intensity of scattered light directly at the rainbow, and strictly zero intensity on the dark side. The Airy integral gives the amplitude (and its square the intensity) near any caustic, including the rainbow. We will discuss this, and some other physical applications in class.

[HW: use the file rain.m to study the dependence on the refraction index, n. When increasing n, when does the rainbow disappear?]

(this is approximately the end of class 1 on special functions)

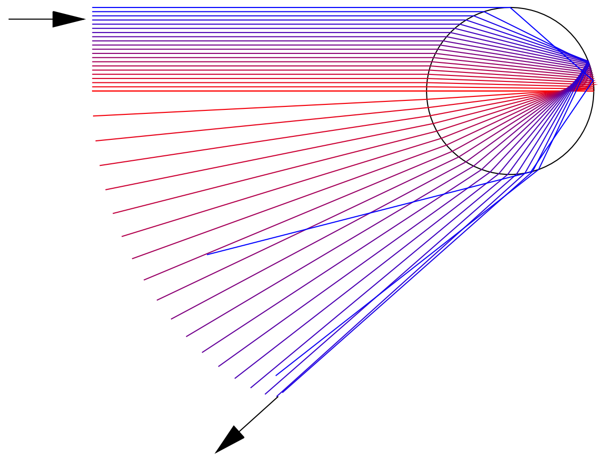

FIG. 3: Formation of a rainbow (geometrical optics). The outgoing arrow indicates the caustic, a direction with infinite intensity. The incoming arrow indicates the rays with the impact parameter of about $0.86R$ (R being the droplet radius), which will form the caustic. A refraction index $n = 4/3$ was used.

Dr. Vitaly A. Shneidman, Phys/MtSE 788, 2nd Lecture

VI. APPLICATIONS OF AIRY FUNCTIONS: THE WKB

Consider the stationary Schrödinger equation

$$u''_{xx} + k^2(x)u = 0 \ , \quad k = \frac{p}{\hbar} \ , \quad p = \sqrt{E - U(x)} \tag{17}$$

with $2m = 1$. Let

$$E > U(x) \text{ for } a < x < b$$

("classically allowed region"). Let

$$u_1(x),\ u_2(x),\ u_3(x)$$

represent solutions for $x < a$, $a < x < b$ and $x > b$, respectively. From previous class,

$$u_1(x) = \frac{C_1}{\sqrt{|p|}} \exp\left(-\int_x^a |k(y)|\ dy\right) \tag{18}$$
$$u_2 = \frac{C_2}{\sqrt{p}} \cos\left[\int_a^x |k|\, dx + \phi\right]$$
$$u_3(x) = \frac{C_3}{\sqrt{|p|}} \exp\left(-\int_b^x |k(y)|\ dy\right)$$

Near a with force $F = -U'(a) > 0$

$$E - U \simeq F(x-a)\ ,\quad |x-a| \ll b-a \tag{19}$$

The integral is evaluated explicitly and one has

$$u_1(x) \simeq \frac{C_1}{\sqrt{F}\,(a-x)^{1/4}} \exp\left[-\frac{2}{3\hbar}\sqrt{F}\,(a-x)^{3/2}\right] \tag{20}$$

This is the asymptote of the left "outer" solution.

To get the inner solution consider

$$u''_{xx} + \frac{1}{\hbar^2}F(x-a)u = 0 \tag{21}$$

Introducing the stretched variable

$$z = \frac{F^{1/3}}{\hbar^{2/3}}(x-a)$$

one gets

$$u''_{zz} + zu = 0 \tag{22}$$

with a solution

$$u^{in}(z) \propto Ai(-z) \tag{23}$$

(the other solution, $Bi(-z)$ has a "wrong" asymptote).

Now we match the inner asymptote as $z \to -\infty$ with eq.(20). This will give a constant - do not find it yet explicitly. Then, the other inner asymptote as $z \to \infty$ will determine u_2. Consider the asymptotes from the first class. Note that the prefactors at $z \to \pm\infty$ look similar, with an extra "2" in denominator. Thus,

$$C_2 = 2C_1\ ,\quad \phi = -\pi/4 \tag{24}$$

(*Kramers'26*).

The above relation is general whether the motion is finite or not (i.e. if b is finite or not). For a finite motion similar arguments can be repeater from the right, giving

$$u_2 = \frac{2C_3}{\sqrt{p}} \cos\left[\int_x^b |k|\,dx - \frac{\pi}{4}\right]$$

This must be the same function, thus $C_1 = \pm C_3$ and

$$\int_a^b k\,dx - \frac{\pi}{2} = n\pi$$

or

$$\oint p\,dx = 2\pi\hbar\left(n + \frac{1}{2}\right) \tag{25}$$

(*Bohr-Zommerfeld*)

Small Project: consider a harmonic oscillator. Write down the WKB approximation explicitly and compare with exact.

Small Project: consider in detail motion in linear potential (when the Airy function solution will be exact). Discuss applications to an electron in a uniform electric field and/or neutrons in gravitational field

VII. REPEATED ERROR INTEGRAL $\mathrm{i^n erfc}$ AND ITS APPLICATIONS

Less know but extremely important special function used both in boundary layer problems (soon) and in solution of the time-dependent diffusion equation.

A. Integer n

Definiton:

$$\mathrm{i^n erfc}(z) = \int_z^\infty \mathrm{i^{n-1}erfc}(t)\,dt \tag{26}$$

$$\mathrm{i^{-1}erfc} = \frac{2}{\sqrt{\pi}}e^{-z^2}\ ,\ \ \mathrm{i^0 erfc}(z) = \mathrm{erfc}(z)$$

Recurrence relations:

$$\mathrm{i^n erfc}(z) = -\frac{z}{n}\mathrm{i^{n-1}erfc}(z) + \frac{1}{2n}\mathrm{i^{n-2}erfc}(z) \tag{27}$$

B. Arbitrary n

Differential equation

$$y''_{zz} + 2zy' - 2ny = 0 \tag{28}$$

$$y = A\mathrm{i^n erfc}(z) + B\mathrm{i^n erfc}(-z) \tag{29}$$

Or

$$\mathrm{i^n erfc}(z) = \frac{2}{n!\sqrt{\pi}} \int_z^\infty (t-z)^n \, e^{-t^2} \, dt \tag{30}$$

with $n! \equiv \Gamma(n+1)$.

C. Asymptotes

1. $z \to -\infty$

Consider eq.(30). One can neglect t compared to z in $(t-z)$. The remainig integral evaluates to $\sqrt{\pi}$. Thus,

$$\mathrm{i^n erfc}(z) \sim \frac{2}{n!}(-z)^n \; , \quad z \to -\infty \tag{31}$$

2. $z \to +\infty$

In eq.(30) the lower limit gives the main contribution. Replacing t by $z+u$ with $t^2 \simeq z^2 + 2uz$ one gets

$$\mathrm{i^n erfc}(z) \sim \frac{2}{\sqrt{\pi}} \frac{e^{-z^2}}{(2z)^{n+1}} \; , \quad z \to \infty \tag{32}$$

Note: there is no $\mathrm{i^n erfc}(z)$ function in *Mathematica*, but it can be expresses through confluent hypergeometric functions in Mathematica 5.2. It is done automatically if the general integral in eq.(30) is evaluated. In later Mathematica 6, 7 and 8 the $\mathrm{i^n erfc}$ can be expressed through a parabolic cylinder function $D_\nu\left[z\sqrt{2}\right]$ - see inerfc7.pdf .

D. A *Mathematica* intermission

we will need a "pure function" - one of the most elegant constructions in Mathematica, similar to an operator in real math. Will introduce in class. In particular, (from previous homeworks) can construct a Wronskian

$$wronsk := FullSimplify[\#1 * D[\#2, x] - D[\#1, x] * \#2]\&$$

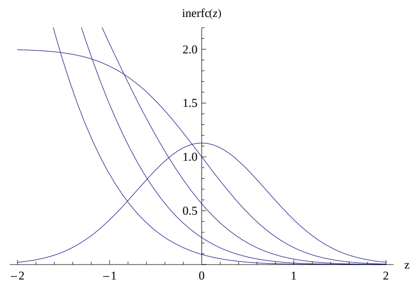

FIG. 4: The $\mathrm{i}^{\mathrm{n}}\mathrm{erfc}(z)$ functions for $n = -1$ (bell-shaped), $n = 0$ (sigmoidal) and $n = 1, 2, 3$ (from top to bottom). For all $n > -1$ note a transition from a power-law asymptote $(-z)^n$ at $z < 0$ to an exponential e^{-z^2}/z^{n+1} at $z > 0$.

(will discuss in class all symbols here).

Now you can try for each pair of linearly independent solutions from the Table:

$$wronsk[Cos[x], Sin[x]]$$

$$wronsk[E^x, E^{(-x)}]$$

$$wronsk[AiryAi[x], AiryBi[x]]$$

$$wronsk[BesselJ[n, x], BesselY[n, x]]$$

Later in the class we will study a package VectorAnalysis, and see that the pure function is really helpful, and is exactly in the spirit of the relevant regular math.

VIII. APPLICATIONS TO THE NUCLEATION PROBLEM

A. The equation

Thermodynamics:

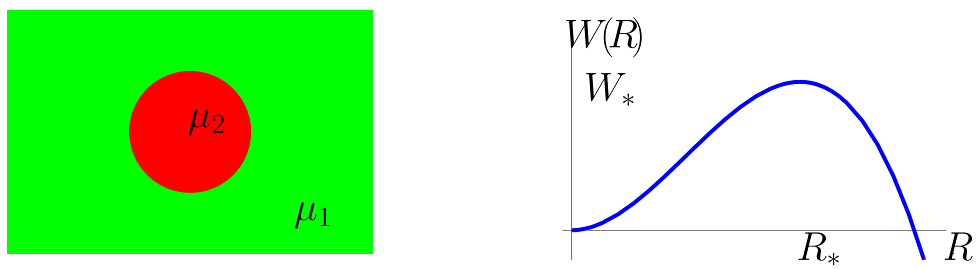

FIG. 5: A nucleus in a supersaturated system with $\mu_1 > \mu_2$ (left) and the minimal work $W(R)$ required to create such a nucleus. The maximum W_* due to excessive interfacial energy determines the barrier to nucleation.

<u>Gibbs</u>: Work to form a nucleus (1878):

$$W(R) = 4\pi R^2\sigma - n(\mu_1 - \mu_2) \ , \quad W_* = \frac{4\pi}{3} R_*^2 \sigma$$

σ - interfacial free energy, $n \propto R^3$ - number of monomers

μ_1, μ_2 - chemical potentials, $(\mu_1 - \mu_2)/k_b T > 0$ - "supersaturation".

KINETICS:

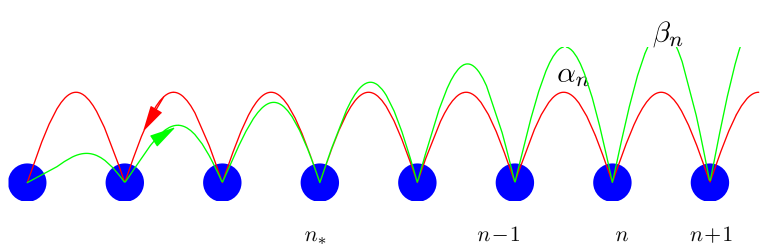

FIG. 6: Classical view of nucleation kinetics. A nucleus performs a random walk in the space of its sizes, n. The gain β_n and loss α_n are size-dependent. Gain "wins" for $n > n_*$, the critical size.

In class:

- Derivation of the kinetic equation
- Connection between random walk and diffusion

Main kinetic ("Becker-Döring") equation:

$$\frac{df_n}{dt} = j_n - j_{n+1} \ , \ \ j_n = \beta_{n-1} f_{n-1} - \alpha_n f_n$$

Gain β_n -from simple kinetic model (e.g., $\beta \propto n^{2/3}$). The loss $\alpha_n = \beta_{n-1} \exp\left[\left(W_n - W_{n-1}\right)/k_B T\right]$ follows from detailed balance.

Continuos approximation:

$$\frac{\partial f}{\partial t} = -\frac{\partial j}{\partial n} \ , \ \ j = -\beta f^{eq} \frac{\partial}{\partial n} \left(\frac{f}{f^{eq}} \right) \tag{33}$$

$$f_n^{eq} \propto \exp\left\{ -\frac{W(n)}{k_b T} \right\}$$

Macroscopic evaluation of β (*Zeldovich (1942)*):

$$\dot{n} = -\frac{\beta}{k_b T} \frac{dW}{dn} \ , \ \ \tau^{-1} = \left. \frac{d\dot{n}}{dn} \right|_*$$

Footnote: Historically, a discrete equation for random walk in the above picture was written first. That equation, however, is somewhat harder to solve and we discuss it after we solve the Zeldovich equation.

We are going to solve the nucleation equation, firts steady-state and then time-dependent using matched asymptotic (singular perturbation) technique. Note: change of variables, both the independent and dependent is an inevitable aspect of the approach. One needs to get used...

Notations:

$$v(n) = \frac{f}{f^{eq}} \ , \ \ \Delta^{-2} = -\left. \frac{1}{2k_b T} \frac{d^2 W}{dn^2} \right|_{n=n_*}$$

We will need the function v since it is smooth (unlike f) at $n < n_*$. The original equation now takes the form

$$\frac{\partial v}{\partial t} = \frac{\partial}{\partial n} \beta \frac{\partial v}{\partial n} + \dot{n} \frac{\partial v}{\partial n} \tag{34}$$

Note that we explicitly identified the deterministic growth rate $\dot{n}$ which will be crucial for subsequent solution. [**Footnote:** Alternatively, one could write equation for f in terms of $\dot{n}$:

$$\frac{\partial f}{\partial t} + \frac{\partial j}{\partial n} = 0 \ , \ \ j = -\beta \frac{\partial f}{\partial n} + \dot{n} f$$

but this is inconvenient for $n < n_*$ where f changes rapidly; f will be more appropriate for the growth region $n > n_*$]

B. Preliminaries: Steady-state solution

This is not the fastest way to get the result, but a good way to introduce ideas of matched asymptotics and to know what to expect on every step of future time-dependent treatment in appropriate limits. [see also the background section in VS, J. Chem. Phys. 115, 8181 (2001)].

One has an ODE:

$$0 = \frac{d}{dn} \beta \frac{dv}{dn} + \dot{n} \frac{dv}{dn} \tag{35}$$

with boundary conditions:

$$v(0) = 1 \ , \ \ v\,(n > n_*) \to 0 \tag{36}$$

Note: it could be tempting to write a "more accurate" $v(1) = 1$, implying at least 1 molecule in a nucleus. At this point, however, this would be an overkill since a continuous description anyway should not be too sensitive to such triffles, and discreteness effects will be discussed separately. More generally, the "0" in $v(0)$ can be understood as any lower boundary $n_{\min}$, and the asymptotic treatment is valid as long as $n_{\min}$ is well below n_*. This can be important, e.g. when comparing with precise numerical solutions of the Becker-Döring equation, where the boundary is often placed at $n_{\min}$ which makes up an appreciable fraction of n_* - see e.g. Kelton, Greer and Thompson, J.Chem. Phys. v. 79, p. 6261 (1983).

Left outer solution $n < n_*$:

$$v(n) = 1$$

Boundary layer:

$$z = \frac{n - n_*}{\Delta} \ , \ \ \dot{n} \simeq \frac{n - n_*}{\tau} = \frac{z\Delta}{\tau}$$

$$v''_{zz} + 2z v'_z = 0 \tag{37}$$

so that

$$v^{in}(z) = \frac{1}{2}\mathrm{erfc}(z)$$

with 1/2 from matching with the outer solution.

Right-hand outer solution: Note that $v\,(z \to \infty)$ decays too fast. It will be inconvenient to match asymptotes. Thus, switch back to smooth $f(n)$ (see previous footnote) One has

$$j = const \equiv j_{st}\ , \quad f_{st}(n) = j_{st}/\dot{n} \tag{38}$$

Flux: from inner solution with $f^{eq} \simeq f_*^{eq} e^{z^2}$

$$j = -\beta f^{eq} v_n' \simeq -\beta_* f_*^{eq} e^{z^2} \frac{1}{\Delta} v_z' = \frac{\beta_* f_*^{eq}}{\Delta\sqrt{\pi}} \tag{39}$$

Note:

$$\beta_* = \frac{\Delta^2}{2\tau}$$

Thus,

$$j_{st} = \frac{\Delta}{2\tau\sqrt{\pi}} f_*^{eq} \tag{40}$$

(*Zeldovich*).

Small project. For steady-state flux can be found exactly. Do that, and evaluate the exact integral asymptotically, as done by Zeldovich. Make a comparative picture

Footnote: Note that the total mass $\int n f_{st}(n)\, dn$ diverges on upper limit. This implies that pure steady-state is impossible at all sizes (particles grow to infinite sizes) and one does need time-dependence. Thus, more accurately, one talks about "quasi-steady-state" before particles grow so big that they start interacting with each other either directly or via depletion of the pool of monomers.

(use a separate handout for a more detailed description and for the transient solution)

IX. ORTHOGONAL POLYNOMIALS

$p_n(x)$ for $-1 \leq x \leq 1$ (will not discuss exceptions, like Hermite). $w(x) \geq 0$ - "weight" (density). "Orthogonality"

$$\int_{-1}^{1} p_n(x) p_m(x) w(x)\, dx\ = 0\,,\ m \neq n$$

Norm

$$||p_n||^2 = \int_{-1}^{1} p_n^2(x) w(x)\, dx$$

Approximation of a function:

$$f(x) = \sum_{n=0}^{\infty} a_n p_n(x) \;, \quad a_n = \frac{1}{||p_n||^2} \int_{-1}^{1} f(x) p_n(x) w(x)\, dx$$

$$f_k^{app}(x) = \sum_{n=0}^{k} a_n p_n(x)$$

$$\lim_{k\to\infty} \int_{-1}^{1} dx \; (f - f_k^{app})^2 \, w = 0$$

("complete set").

A. Examples

<u>Legendre</u>: $P_n(x)$, with $w(x) \equiv 1$.

Norm

$$||P_n||^2 = 2/(2n+1)$$

First five:

$$\begin{aligned}
&1 \\
&x \\
&\tfrac{1}{2}\,(3x^2 - 1) \\
&\tfrac{1}{2}\,(5x^3 - 3x) \\
&\tfrac{1}{8}\,(35x^4 - 30x^2 + 3) \\
&\tfrac{1}{8}\,(63x^5 - 70x^3 + 15x)
\end{aligned}$$

<u>Chebyshev</u>: $T_n(x)$ with $w(x) = 1/\sqrt{1-x^2}$.

Norm

$$||T_n||^2 = \frac{\pi}{2}\,, n \neq 0\,; ||T_0||^2 = \pi$$

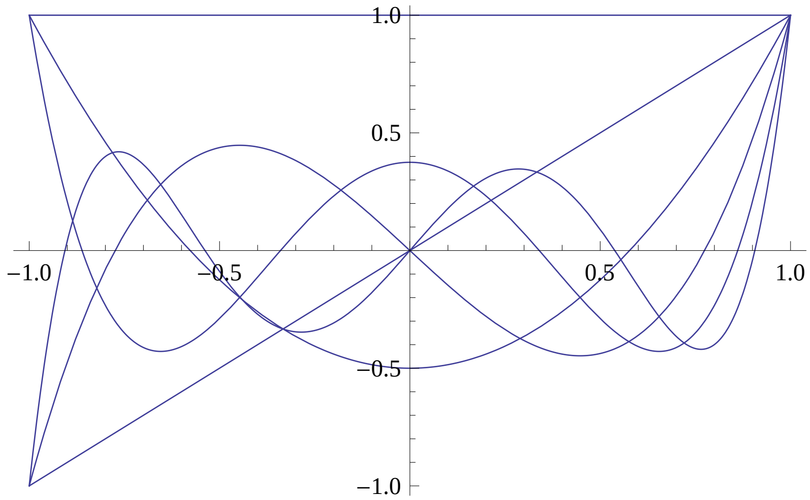

FIG. 7: First 5 Legendre polynomials

First 5:

$$
\begin{aligned}
&1 \\
&x \\
&2x^2 - 1 \\
&4x^3 - 3x \\
&8x^4 - 8x^2 + 1 \\
&16x^5 - 20x^3 + 5x
\end{aligned}
$$

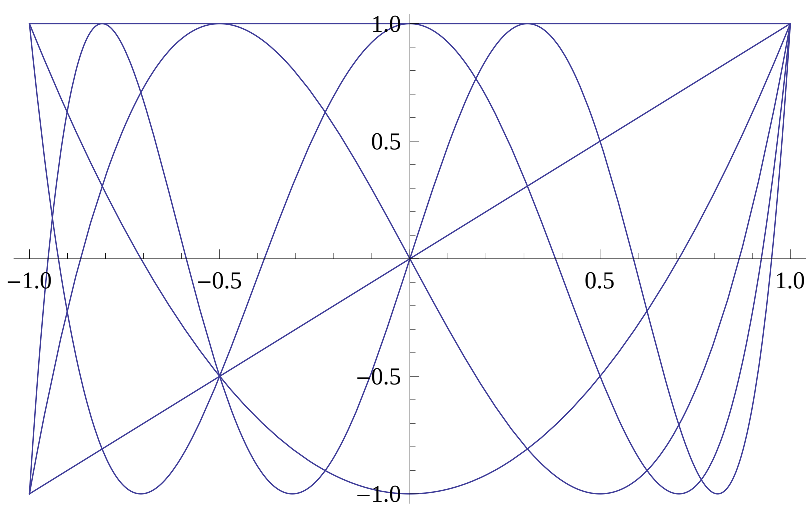

FIG. 8: First 5 Chebyshev polynomials

Differential equation and trigonometric representation:

$$\left(1-x^2\right)T''-xT'+n^2T=0$$

Let

$$x=\cos\theta\,,\ \frac{d}{dx}=-\frac{1}{\sin\theta}\frac{d}{d\theta}$$

then

$$\frac{d^2T}{d\theta^2}+n^2T=0$$

and

$$T_n=\cos(n\theta)=\cos(n\arccos x)$$

<u>Error</u>

$$e_k(x)=f(x)-f_k^{app}(x)$$

see 788_orthog.pdf for $f=\sin\pi x$.

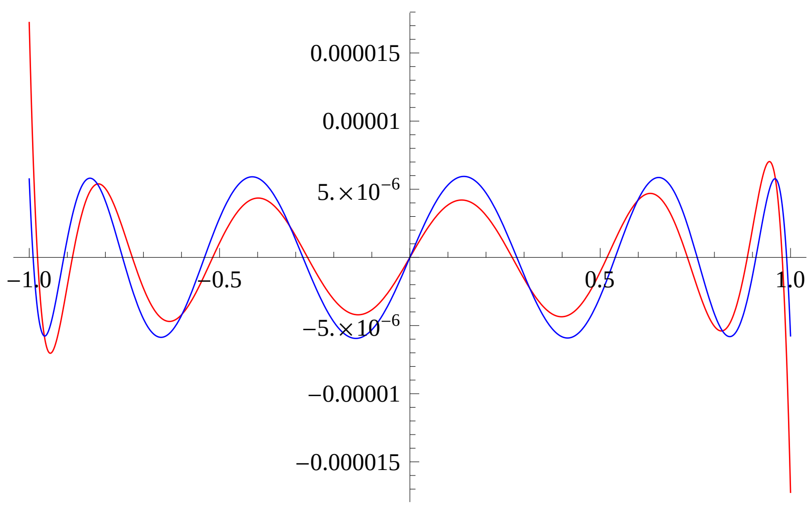

FIG. 9: Error of 10-term approximation of $\sin\pi x$. Red - with Legendre polynomials, blue - with Chebyshev. Note that Legendre is worse near the edges.

X. OVERVIEW OF OTHER SPECIAL FUNCTIONS

Easier to classify for a full form of ODE:

$$f(x)y'' + g(x)y' + h(x)y = 0$$

[Transformation to "normal" form of a differential equation is achieved by changing variables in order to get rid of the 1st derivative:

$$u(x) = y(x)\exp\left\{\frac{1}{2}\int (g/f)dx\right\}$$

will give

$$u'' + I(x)u = 0\,,\ I(x) = \frac{h}{f} - \frac{1}{4}\left(\frac{g}{f}\right)^2 - \frac{1}{2}\left(\frac{g}{f}\right)'$$

HW: check this. If you are good with Mathematica write a pure function which calculates $I(x)$ for any f, g, h]

Wronskian W. Taking the derivative of the definition of W and replacing the 2nd derivatives using the original differential equation, one obtains

$$W' = -(g/f)W$$

Then:

$$W = \exp\left\{-\int (g/f)dx\right\}$$

Note: for a full form of ODE generally

$$W(x) \neq const$$

Classification: number of free parameters in $f(x), g(x), h(x)$ - see next page.

Name	$f(x)$	$g(x)$	$h(x)$	Applications	*Mathematica*
sin, cos	1	0	1	everywhere	Sin, *Cos*
$\exp(\pm x)$	1	0	-1	everywhere	Exp
Airy	1	0	-x	Optics (caustics), QM: transition to classically forbidden region; motion in constant field	AiryAi, AiryBi
$\mathrm{i^n erfc}(\pm x)$	1	$2x$	$-2n$	diffusion-type (heat conductivity)	-
Bessel (modified Bessel)	x^2	x	$\pm x^2 - n^2$	(mostly) problems with cylindrical symmetry	BesselJ, BesselY ($-$) or BesselI, BesselK ($+$)
Legendre	$1 - x^2$	$-2x$	$n(n+1)$	problems with symmetry close to spherical	LegendreP, LegendreQ
Hermite	1	$-2x$	$2n$	QM: harmonic oscillator	HermiteH
Chebyshev	$1 - x^2$	$-x$	n^2	approximating polynomials	ChebyshevT, ChebyshevU
Confluent hypergeometric	x	$c - x$	$-a$	very broad	see Hypergeometric
Mathiew	1	0	$a - q\cos(2x)$	parametric resonance, stability of non-linear oscillations	MathieuC, MathieuS
Hypergeometric	$x(x-1)$	$c - (a + b + 1)x$	$-ab$	TOO broad	see Hypergeometric

HW: *Bring the equation for Chebyshev polynomials to a normal form. Plot a few polynomials $T_n(x)$ on a single plot.*

HW: *using the fact that $T_n(x)$ are orthogonal on the interval $[-1, 1]$ with a weight function $w(x) = 1/\sqrt{1-x^2}$, expand $f(x) = \sin(\pi x)$ as $f^{app} \simeq \sum_0^N a_n T_n(x)$ for some modest N. Plot the error $f - f^{app}$. Do a similar expansion (same N) using Legendre polynomials and compare the error plots.*

A. Why special functions in Physics?

Laplace operator:

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\ , \quad \text{i.e. } \Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

Main equations with Δ:

- Laplace equation

  $$\Delta\phi = 0$$

  ϕ - electrostatic potential (in empty space), gravitational potential, etc.

- Poisson equation

  $$\Delta\phi = -\rho/\epsilon_0\ , \quad \rho\ -\ \text{charge density}$$

- Diffusion equation

  $$\Delta\phi = D^{-1}\frac{\partial\phi}{\partial t}$$

  ϕ - concentration (or temperature in heat conductivity problem), D- diffusion coefficient

- Wave equation

  $$\Delta\phi = \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2}\ , \quad c\ -\ \text{wave speed}$$

- Schrödinger equation

  $$-\frac{\hbar^2}{2m}\Delta\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}\ , \quad \Psi\ -\ \text{wave function}$$

If all PDE why talk ODE? - Separation of variables. For example, look for a solution

$$\phi = \Phi\left(\vec{r}\right)e^{-\lambda t}$$

(diffusion) or

$$\phi = \Phi e^{i\omega t}$$

(wave equation). Both will give a Helmgolz equation

$$\Delta\Phi + k^2\Phi = 0$$

with $k^2 = \lambda$ (diffusion) and $k^2 = \omega^2/c^2$ (wave). Similarly, the Shrödinger equation, $k^2 = (E - V)2m\hbar^2$.

Now still a PDE (x, y, z), but if **symmetry** Φ depends only on r. For spherical $(d = 3)$, circular $(d = 2)$ etc. systems of coordinates

$$\Delta = \frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} + \text{angul.part}$$

Now for $d = 2$ and only r-dependence

$$\Delta\Phi(r) = \frac{d^2\Phi}{dr^2} + \frac{1}{r}\frac{d\Phi}{dR}$$

typical Bessel.

On the o.h., for $d = 3$ the angular part leads to Legendre polynomials.

XI. BESSEL FUNCTIONS

Bessel functions are the most "popular" in physics, but we will also use them to illustrate some general features of the special functions which were not seen in the simpler, Airy functions.

The singular point is $x = 0$. So, $y_1(x) = J_n(x)$ -first kind, and $y_2(x) = Y_n(x)$ - second kind, see Fig. 10. [HW: using Mathematica, calculate the Wronskian, $W[J_n(x), Y_n(x)]$; compare with general predictions]. Let us transform to normal form:

$$u(x) = y(x) \exp\left\{\frac{1}{2}\int (x/x^2)dx\right\}$$

or

$$u(x) = y(x)\sqrt{x}$$

and

$$I(x) = 1 - n^2/x^2 + 1/4x^2$$

Note that for large x the function $I(x)$ approaches 1. Thus, according to WKB, $u(x)$ for $x \gg 1$ is oscillatory, with period 2π and constant amplitude, while $y(x)$ oscillates with amplitude decaying as $1/\sqrt{x}$. Indeed, one has:

A. Asymptotes

$$J_n(x) \sim \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{1}{2}n\pi - \frac{\pi}{4}\right) \tag{41}$$

and

$$Y_n(x) \sim \sqrt{\frac{2}{\pi x}} \sin\left(x - \frac{1}{2}n\pi - \frac{\pi}{4}\right) \tag{42}$$

[HW: plot a few Bessel functions together with their asymptotes].

For large n the Bessel function will be non-oscillatory for a large interval of x (since $I(x)$ will be negative). For large n and *finite* x one can use the small-x expressions described below. More interesting is the case when both x and n are large, when transition to oscillations is expected for $x \sim n$. Here one recovers a relation between the Bessel functions and the Airy functions - see Abramowitz, 9.3.4, etc.

[HW: Plot $J_n(x)$, $Y_n(x)$ for a reasonably large n. Note: in some cases you will need some finite interval of x around the "transition value" of $x = n$, otherwise the relative value of the function can be too large or too small to plot on the same scale.
Small project: plot on the same scale the Airy-function approximation from Abramowitz]

B. Small x

Near the singular point and for $n \neq 0$ one can neglect x^2 in the free term. This leads to what is known as a *homogeneous* equation which can be solved by a power-law. We look for a solution $y(x) \propto x^\mu$, and get

$$\mu(\mu - 1) + \mu - n^2 = 0$$

or

$$\mu = \pm n$$

Indeed, one has for $x \to 0$

$$J_n \sim \left(\frac{x}{2}\right)^n \frac{1}{\Gamma(n+1)}\ , \quad n \geq 0 \tag{43}$$

and

$$Y_n \sim -\frac{1}{\pi}\left(\frac{x}{2}\right)^{-n} \Gamma(n)\ , \quad n > 0 \tag{44}$$

A special case is

$$Y_0(x) \sim \frac{2}{\pi}\left[\ln\frac{z}{2} + \gamma\right]\ , \quad \gamma = 0.5772... \tag{45}$$

Why logarithmic singularity? - from Wronskian!

C. Integer vs. non-integer n, generating function, recurrence relations and integral representation

For non-integer $n = \nu$ the solution $J_{-\nu}$ is linearly independent from J_ν. In particular, there exists a formula expressing Y_ν through J_ν and $J_{-\nu}$ (see, e.g., Abramowitz, 9.1.2). For integer n such solutions are not independent:

$$J_{-n}(x) = (-1)^n J_n(x) \tag{46}$$

This follows from the so-called *generating function*

$$e^{x/2(t-1/t)} = \sum_{n=-\infty}^{n=\infty} J_n(x) t^n \tag{47}$$

(note: here n are strictly integer!). Many recurrence relations which can be obtained directly from the above equation, e.g.

$$J_{n-1} - J_{n+1} = 2J_n' \tag{48}$$

From here, and from the symmetry relation, one gets

$$J_0' = -J_1$$

. Another relation is

$$J_n(x) = x^{-n} \int^x z^n J_{n-1}(z) dz \tag{49}$$

There are several integral representations, the "best" is

$$J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{ix \sin\theta} d\theta \tag{50}$$

which is famous for optics applications. (A similar expression for any n is available - see Abramowitz).

D. Fraunhofer diffraction

Physics will be discussed in class. A circular aperture of diameter $D = 2a$ is considered, and the amplitude Φ is evaluated in the direction α from the center of the apperture for small α. The field intensity is proportional to $|\Phi|^2$.

From Huygens principle one needs and integral over the opening of the apperture ($\vec{r}$ being the vector from the center to any point in the plane of the apperture)

$$\int \exp\left(-ikR\right) d\vec{r}$$

$\vec{R}$ is the vector connecting the point and the observation point.

If $\vec{R}_0$ is the vector from the center to the observation point, one has

$$\vec{r} + \vec{R} = \vec{R}_0$$

and for $r \ll R_0$

$$R \simeq R_0 - \frac{\vec{R}_0 \cdot \vec{r}}{R_0}$$

If θ is the angle $\vec{r}$ makes in the plane of the apperture, then

$$\vec{R}_0 \cdot \vec{r} = R_0 \sin\alpha r \cos\theta$$

thus

$$R \simeq R_0 - r\cos\theta\sin\alpha$$

The constant in the phase does not matter (Why?) and one has

$$\Psi\left(\alpha\right) \propto \int_0^a rdr \int_0^{2\pi} \exp\left(-ikr\cos\theta\sin\alpha\right) d\theta = 2\pi \int_0^a J_0\left(rk\sin\alpha\right) rdr = \frac{2\pi}{k^2\sin^2\alpha} \int_0^{ak\sin\alpha} J_0(x)xdx$$

This is

$$\frac{2\pi}{k^2\sin^2\alpha} J_1\left(ak\sin\alpha\right) \cdot \left(ak\sin\alpha\right)$$

For intensity one thus gets ($\lambda = 2\pi/k$):

$$\Phi^2 \propto \frac{1}{\sin^2\alpha} J_1^2\left[\frac{\pi D\sin\alpha}{\lambda}\right] \tag{51}$$

(λ is the wavelength). For small α one can replace $\sin\alpha$ by α, and the result is shown in Fig. 11.

HW: *Compare the numerical values of intensities at the 1st and 2nd maximum relative to the primary maximum at* $\alpha = 0$

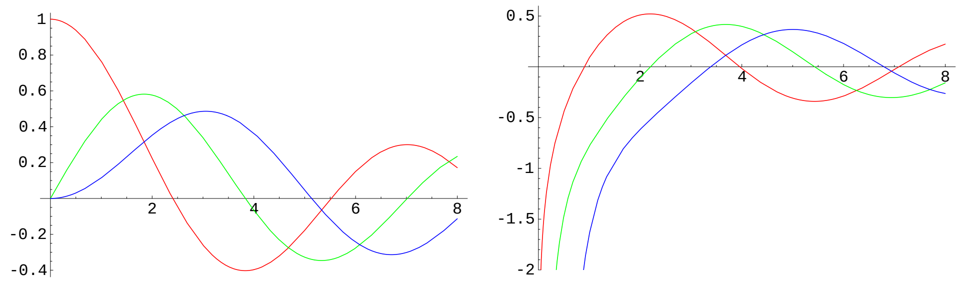

FIG. 10: Bessel functions $J_n(x)$ (1st kind) and $Y_n(x)$ (2nd kind) for $n = 0$ (red), $n = 1$ (green) and $n = 2$ (blue).

E. Small projects with Bessel functions

(optional - ask for references) :

1. examine the vibration eigenmodes of a circular membrane; see figures below, and the 788_BesselDrum.nb; some physics will be discussed in class
2. examine wave propagation in a cylindrical waveguide
3. study the spherical Bessel functions, $J_{n+1/2}$, etc., and consider a quantum particle in a spherical box.]

F. Modified Bessel functions

Note that going from x^2 to $-x^2$ in the Bessel equation can be achieved by going from x to ix. Strictly speaking, great care must be shown since we (i.e., us) do not know well enough analytical properties in the complex plain. Nevertheless,

$$I_n(x) = (-i)^n J_n(ix) \tag{52}$$

will be a real-value function, with the same asymptotes as J_n for $x \to 0$, but with an exponential growth as $x \to \infty$

$$I_n(x) \sim e^x/\sqrt{2\pi x} \tag{53}$$

One can expect that a similar construction will be used starting from $Y_n(x)$. Unfortunately, there is an extra factor $\pi/2$ (you can notice it by comparing wronskians). The

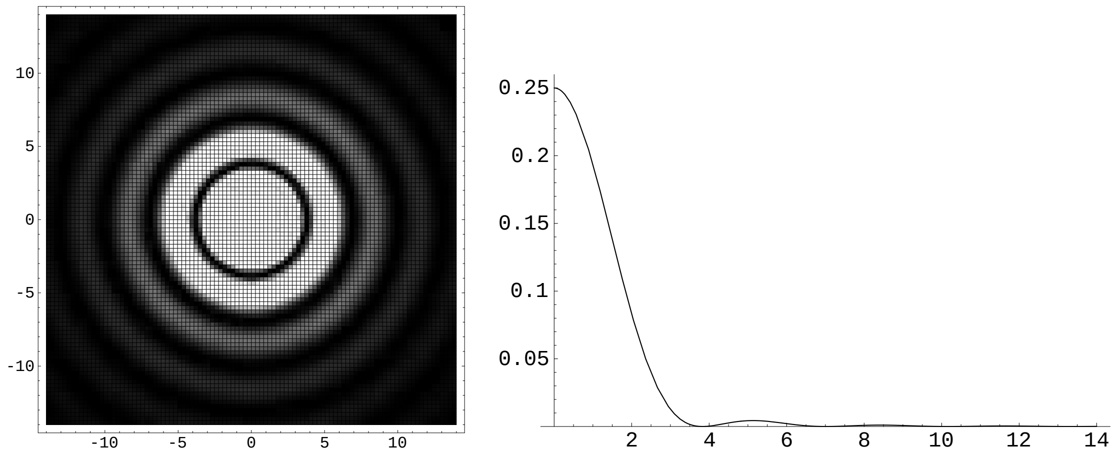

FIG. 11: Fraunhofer diffraction from a circular aperture with diameter D. The arguments are $\alpha\pi D/\lambda$ with $\alpha \ll 1$ being the angle and λ the wavelength. The angle to see the first minimum is called the *angular resolution*, $\theta \approx 1.21967\lambda/D$. Note that the intensity is very small beyond the first minimum (right figure), but still can be easily picked up by the eye (left figure). [Also, note: in optics literature this circular pattern is sometimes called "Airy disc" - has nothing to do with Airy functions. The bright spot at the center is called the "Poisson spot".]

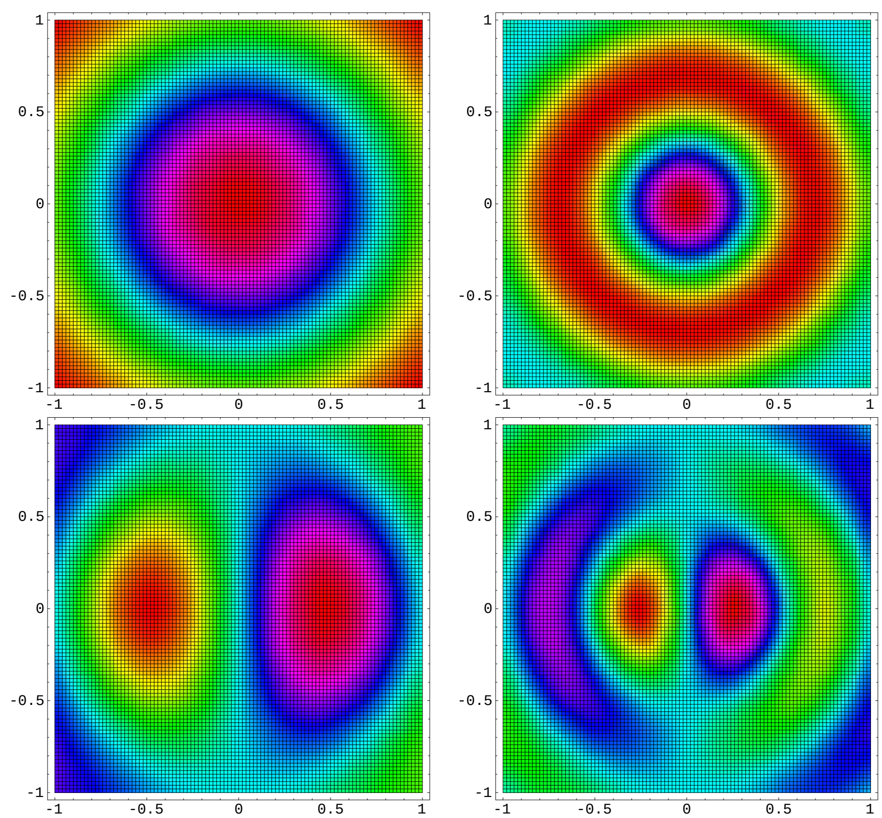

FIG. 12: Normal modes for a vibrating membrane of radius 1.

power-law asymptotes of $K_n(x)$ ($n \neq 0$) as $x \to 0$ remain similar to those of $Y_n(x)$, but with this extra factor. For $n = 0$ one has

$$K_0(x) \sim -\ln(x/2) - \gamma \ , \quad x \to 0 \tag{54}$$

Alternatively, for $x \to \infty$ and any n one has

$$K_n(x) \sim e^{-x}/\sqrt{2\pi x} \cdot \pi/2 \tag{55}$$

The general structure of the functions is shown in Fig. 13. Note that all functions are now positive. Unlike the regular Bessel case, there are now no "good" functions which remain finite for both $x = 0$ and $x \to \infty$. But this can be quite "physical" , see the example below.

HW: *Calculate the Wronskian of I_n, K_n using Mathematica for several different n*

HW: *Plot a few modified Bessel functions together with their asymptotes .*

G. Diffusion of neutrons

Physics will be discussed in class. Consider a stationary problem

$$D\Delta\phi - \sigma\phi = 0 \tag{56}$$

with cylindrical symmetry. We now switch to cylindrical coordinates where expect dependence on r only:

$$r^2\phi'' + r\phi' - r^2k^2\phi = 0 \ , \quad k^2 = \sigma/D \tag{57}$$

[You can check this with Mathematica:

<<"Calculus‘VectorAnalysis‘"

$$FullSimplify[Laplacian[u[r], Cylindrical[r, t, z]]]$$

(with t standing for *theta*, but since we neglect the dependence on t and z it does not matter anyway)

HW: try this]

The equation (57) is solved as

$$c_1 I_0(kr) + c_2 K_0(kr)$$

(again, if you need help, use Mathematica:

$$l := r^2 * D[\#, r, r] + rD[\#, r] - k^2 r^2 \#\&$$

gives the operator and

$$DSolve[l[u[r]] == 0, u[r], r]$$

gives the above general solution - try this!)

Now you can see, that whatever we try, there will be an infinity. What that means? Will discuss in class - the infinity at $r = 0$ does matter, see Fig. 14. Also note, cannot use $\sigma = 0$, i.e. in 2-dimensions (and in 1-dim.) there is NO steady-state diffusion in infinite space. 3D is different, however.

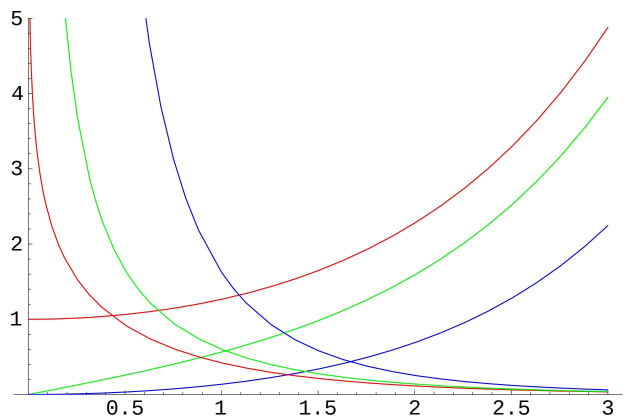

FIG. 13: Modified Bessel functions of the 1st kind , $I_n(x)$ (ascending lines) and 2nd kind, $K_n(x)$ (descending lines) for $n = 0$ (red), $n = 1$ (green) and $n = 2$ (blue).

What infinity at $r = 0$ means? Need a source! Flux (density):

$$j = -D\frac{d\phi}{dr} = -c_2 \frac{dK_0(kr)}{dr}$$

Total flux (per unit length in the z-direction)

$$J(r) = 2\pi r j(r)$$

and the intensity of source:

$$S_0 = \lim_{r \to 0} J(r) = 2\pi D c_2$$

which gives c_2 if source is known.

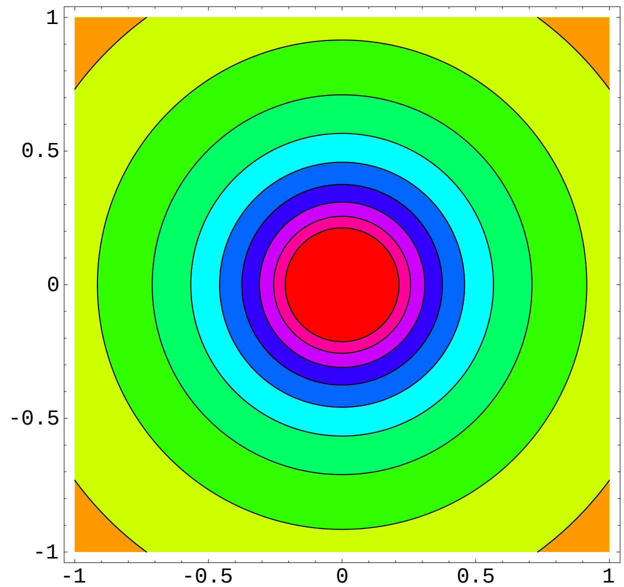

FIG. 14: Concentration profiles for the steady-state diffusion of neutrons. Note a singularity (red cented) near $r = 0$.

Dr. Vitaly A. Shneidman, Phys/MtSE 788, 6th Lecture

XII. ELECTROSTATICS AND LEGENDRE POLYNOMIALS

The Legendre polynomials are related to the Laplace operator in spherical coordinates (its angular part - see below) and thus have an enormous amount of applications in Physics. However, electrostatics provides a very natural way to introduce them, and provides us with important intuition.

A. Field of point charges and the generating function for Legendre polynomials (LP)

Consider a point charge q placed on the z-axes at a distance a from the origin (figure will be shown in class). We are interested in the electrostatic potential produced by this charge at an observation point at a distance r from the the origin (not from this charge!), which is seen at an angle θ. If the distance from the charge is r_1, then the potential is

$$\phi = kq/r_1 \ , \quad k \approx 9 \cdot 10^9 Nm^2/C^2 \equiv 1/(4\pi\epsilon_0)$$

From geometry,

$$r_1^2 = r^2 + a^2 - 2ar\cos\theta$$

Consider now $r \gg a$ and perform a series expansion of the potential in powers of a/r. The coefficients of this expansion are functions of $\cos\theta$ and *by definition* they correspond to Legendre polynomials. More precisely:

$$\frac{1}{\sqrt{r^2 + a^2 - 2ar\cos\theta}} = \frac{1}{r}\sum_{n=0}^{\infty} P_n(\cos\theta)\left(\frac{a}{r}\right)^n$$

Here P_n are known are the "Legendre polynomials" (LP), and the function on the left is the "generating function". (Of course we can replace $\cos\theta$ by x, but it is useful to remember the connection).

[HW: use the Series command in Mathematica to get the first 5 LP]

Consider now a dipole with charges $\pm q$ at $\pm a$. The even terms of the expansions get cancelled, while the odd double. One has

$$\phi(r,\theta) = \frac{2kq}{r}\left\{P_1(\cos\theta)\left(\frac{a}{r}\right) + P_3(\cos\theta)\left(\frac{a}{r}\right)^3 + \ldots\right\}$$

Here $2aq = d$ is the dipole moment, so that for $r \to \infty$

$$\phi \approx \frac{kdP_1(\cos\theta)}{r^2}$$

Similarly, the procedure can be continued by making a more symmetric distribution of charges with $d = 0$ (e.g., $+q$ at $\pm a$ and $-2q$ at 0), and considering the leading term for $r \gg a$ which is due to the quadrupole moment, etc.

B. Explicit expressions and recurrence relations

For small n LP are simple:

$$P_0(x) = 1\ ,\ \ P_1(x) = x\ ,\ \ P_2(x) = \left(3x^2 - 1\right)/2\ldots$$

(see section on Orthogonal polynomials for more). There are many recurrence relations which allow to generate LP fast, without the actual series expansion, e.g.

$$(n+1)P_{n+1}(x) = x(2n+1)P_n(x) - nP_{n-1}(x)$$

[HW: Use the above recurrence relation, and start with P_0, P_1 to obtain other LP. For some reasonably large n compare with standard LegendreP in Mathematica, and compare the evaluation time using the Timing command. Do not try to view the polynomial on the screen for large n !].

Note that

$$P_n(1) = 1 \ , \quad P_n(-1) = (-1)^n$$

this follows, e.g. from the recurrence relation [HW (optional) show this]. Also

$$P_{-n}(x) = P_{n-1}(x)$$

[HW: check this using FullSimlify]

C. Relation to Laplacian

In spherical coordinates one has

$$\hat{\Delta} = \hat{\Delta}_R - \frac{1}{r^2}\hat{l}^2$$

with l^2 given by

$$\hat{l}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

[HW: (optional) check this using Calculus‘VectorAnalysis‘) Making a substitution

$$x = \cos\theta \ , \quad \sin^2\theta = 1 - x^2$$

one gets an equation

$$\hat{l}^2 = -\frac{\partial}{\partial x}\left[\left(1-x^2\right)\frac{\partial}{\partial x}\right] - \frac{1}{1-x^2}\frac{\partial^2}{\partial\phi^2}$$

which leads for LP in x (or in $\cos\theta$) if $\frac{\partial^2}{\partial\phi^2} = 0$.

Another relation

$$\hat{\Delta} r^n P_n(\cos\theta) = 0 \text{ for any } n$$

[HW (optional): check this using Calculus‘VectorAnalysis‘] I.e. in problems with no dependence on ϕ an expansion in $r^n P_n(\cos\theta)$ with $-\infty < n < \infty$ is possible. We will use it in the problem of a conducting sphere in a uniform field.

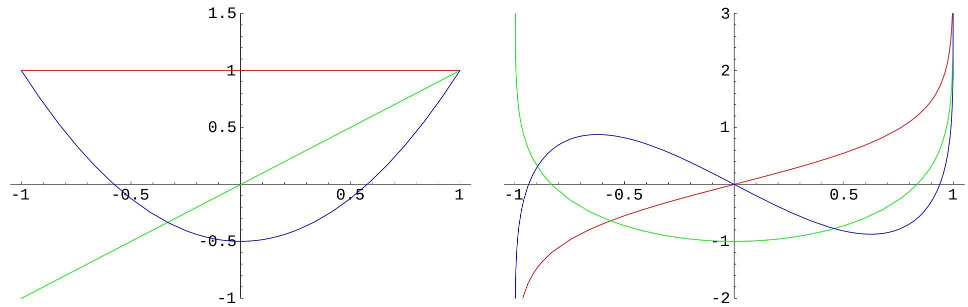

FIG. 15: Legendre polynomials $P_n(x)$ (left) and Legendre functions of the 2d kind, $Q_n(x)$ (right) for $n = 0, 1, 2$

D. The other solution

Consider now the differential equation for the LP - see Table. There are singular points at $x = \pm 1$. The LP are solutions of the 1st kind, which are regular. The other solutions are the Legendre function of the 2d kind, $Q_n(x)$. They are *not* polynomials (why?), and are given by LegendreQ in Mathematica. Both types of solutions are shown in Fig. 15. The functions $Q_n(x)$ have logarithmic singularities, e.g.

$$Q_0(x) = \frac{1}{2}\ln\frac{1+x}{1-x}\ , \quad Q_1(x) = \frac{1}{2}x\ln\frac{1+x}{1-x} - 1\ , \ldots$$

[HW (optional): using Mathematica check for some n, or in general, that Q_n satisfy the same recurrence relation as P_n.]

E. Physical applications

1. *Gravitational field*

$$U\left(r,\theta\right) = \frac{GM}{R}\left[\frac{R}{r} - \sum_{n=2}^{\infty} a_n \left(\frac{R}{r}\right)^{n+1} P_n\left(\cos\theta\right)\right]$$

Why no a_1?

$$a_2 \sim 10^{-3}\ , \quad a_3 \sim 2.5\cdot 10^{-6}\ \ldots$$

Will discuss in class the non-spherical corrections to gravitational field of Earth. [Small project: Plot the direction of $\vec{g}$ compared to the "vertical" as a function of r, θ.]

[Large project: Study the motion of a satellite. Note: will need to integrate Newtons equations in spherical coordinates, ask for references].

2. Conducting sphere in uniform field $\vec{E}_0$

Small project. Physics will be discussed in class.

$$r^n P_n(\cos\theta)$$

is the solution of the Laplce equation for any n. From the recurrence relations

$$P_{-n}(x) = P_{n-1}(x)$$

Thus

$$V(r,\theta) = \sum_{n=0}^{\infty} \left\{ a_n r^n P_n(\cos\theta) + b_n \frac{P_n(\cos\theta)}{r^{n+1}} \right\}$$

Boundary condition (1st one):

$$V(r \to \pm\infty) = \mp E_0 r \cos\theta$$

Thus,

$$a_1 = -E_0\ , \quad a_n = 0 \text{ for } n \neq 1$$

2nd BC:

$$V(r = R) = 0$$

(uncharged sphere). Thus

$$b_0/R + \left(\frac{b_1}{R^2} + a_1 R\right) P_1(\cos\theta) + \sum_{n=2}^{\infty} b_n \frac{P_n(\cos\theta)}{r^{n+1}} = 0$$

Thus,

$$b_1 = -a_1 R^3 = E_0 R^3\ , \quad b_n = 0 \text{ for } n \neq 1$$

or

$$V(r,\theta) = -E_0 r P_1(\cos\theta)\left(1 - (R/r)^3\right)$$

Charged sphere: $V(R) = Q/R$ (CGS). Thus, $b_0 = Q$ and Q/r is added to previous solution at $r \geq R$ (superposition!)

Plotting of lines is in condSphere.m. The result is in Fig. 16

[Small projects (optional): reproduce the plots using StreamLine plot]

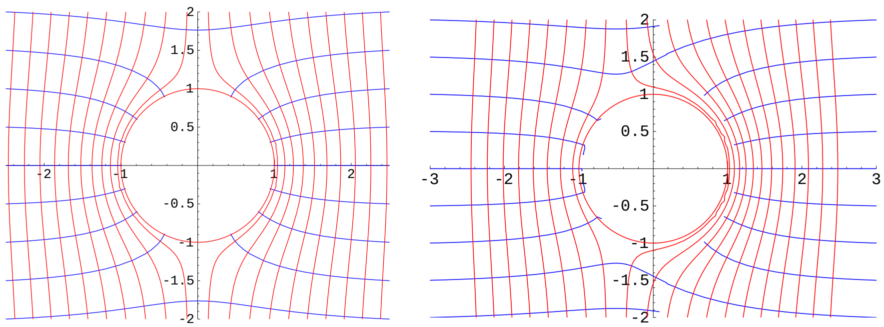

FIG. 16: Left: Electric field lines (blue) and equipotential surfaces (red) for a conducting sphere in a uniform field. Right: same, when the sphere is charged wit a positive charge

3. *Dielectric sphere*

The expansion (**??**) is the same, but now *out* and *in* (use capital A_n and B_n to distinguish). Out, the same BC at $r \to \infty$. Thus,

$$A_1^{out} = -E_0 \ , \ \ A_n^{out} = 0 \text{ for } n \neq 1$$

Inside - no singularity at $r = 0$:

$$B_n^{in} = 0$$

Boundary conditions on the surface: $\vec{E}_{||}$ continuous (otherwise circulation $\neq 0$)

D_{normal} continuous; $\vec{D}^{in,out} = \kappa_{1,2}\vec{E}^{in,out}$.

Thus

$$-\frac{1}{R}\frac{\partial V^{in}(R,\theta)}{\partial\theta} = -\frac{1}{R}\frac{\partial V^{out}(R,\theta)}{\partial\theta}$$

and

$$-\kappa_1\frac{\partial V^{in}(r=R,\theta)}{\partial r} = -\kappa_2\frac{\partial V^{out}(r=R,\theta)}{\partial r}$$

From these BC:

$$A_1^{in} = A_1^{out} + B_1^{out}/R^3$$

and

$$\kappa_1 A_1^{in} = \kappa_2\left(A_1^{out} - 2B_1^{out}/R^3\right)$$

(linear system of equations). Thus,

$$A_1^{in} = -\frac{3\kappa_2}{2\kappa_2+\kappa_1}E_0 \ , \ \ B_1^{out} = \frac{\kappa_1-\kappa_2}{\kappa_1+2\kappa_2}$$

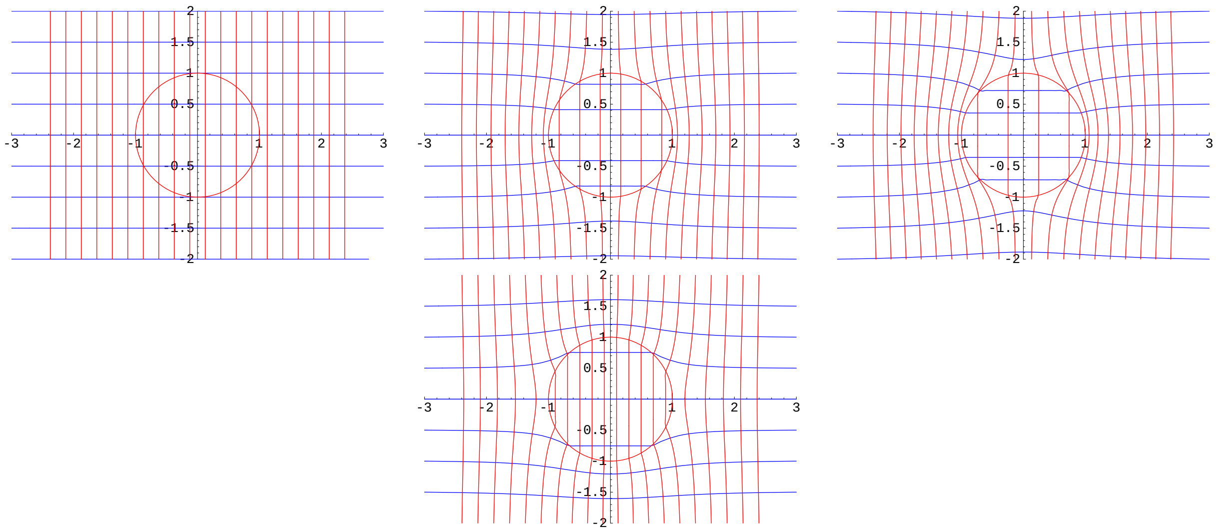

FIG. 17: Electric field lines (blue) and equipotential surfaces (red) for a dielectric sphere in a uniform field. $\epsilon \equiv \kappa^{in}/\kappa^{out}$; from top left, clockwise: $\epsilon = 1$ (test); $\epsilon = 2$, $\epsilon = 4$ and $\epsilon = 0.33$ (cavity in a dielectric). Note that the field lines better represent the vector $\vec{D}$, rather than $\vec{E}$. (Think why?)

and

$$V^{in} = -\frac{3\kappa_2}{2\kappa_2 + \kappa_1} E_0 r \cos\theta$$

$$V^{out} = -E_0 r \cos\theta + \frac{\kappa_1 - \kappa_2}{\kappa_1 + 2\kappa_2} E_0 \frac{R^3}{r^2} \cos\theta$$

Checkpoint1: $\kappa_1 = \kappa_2$:

$$V^{in} = V^{out} = -E_0 r \cos\theta$$

Checkpoint2: $\kappa_1/\kappa_2 \to \infty$:

$$V^{in} = 0\ , \quad V^{out} = -E_0 r \cos\theta \left(1 - \frac{R^3}{r^3}\right)$$

(conductor).

General:

$$E^{in} = \frac{3\kappa_2}{2\kappa_2 + \kappa_1} E_0$$

Uniform field!!!

Part III

Diffusion

XIII. THE DIFFUSION APPROXIMATION TO RANDOM WALK

Consider a "distribution function" f_k with $k = 0, \pm 1, \pm 2, \ldots$ (analog of $2m - n$) which changes with "time" t, analog of n. One has

$$\begin{aligned} f_k(t+1) &= f_k(t) + \frac{1}{2} f_{k-1}(t) + \frac{1}{2} f_{k+1}(t) - f_k \\ &= f_k(t) + D\left[f_{k-1}(t) + f_{k+1}(t) - 2f_k(t)\right] \ , \quad D = 1/2 \end{aligned} \tag{58}$$

Considering $f_k(t)$ as a smooth function of both t and k, one has (with k replaced by x):

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2} \tag{59}$$

The solution ("Greens function") is given by

$$G(x,t) = \frac{1}{2\sqrt{\pi D t}} \exp\left\{-\frac{x^2}{4Dt}\right\} \tag{60}$$

Correspondence with the exact solution is excellent - see Fig. 18.

A. Biased diffusion

Consider a biased random walk with probability p going right, and $q = 1 - p$ going left on every step.

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2} + v \frac{\partial f}{\partial x} \ , \quad v = p - q \tag{61}$$

HW: derive this, an generalize the exact expression.

The Green's function just drifts with time

$$G_b(x,t) = G(x - vt, t)$$

HW: check this

Again, correspondence is excellent - see Fig. 19.

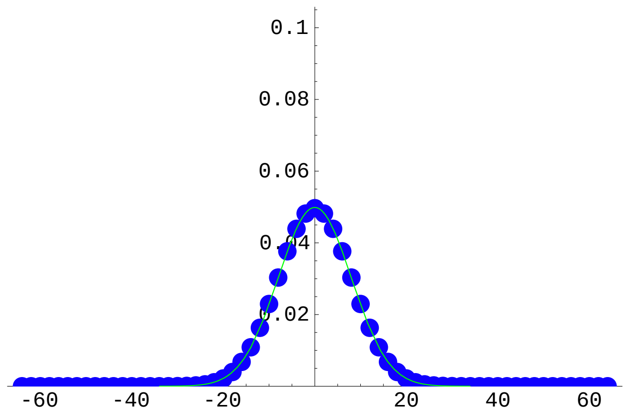

FIG. 18: Non-biased random walk (points) and the diffusion approximation

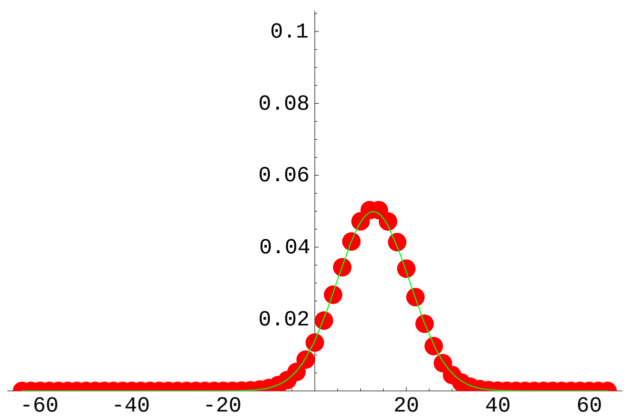

FIG. 19: Same, for a biased random walk.

B. Limitations of the diffusion description

Note that the exact expression is strictly zero for $2m - n > n$, but the diffusion gives a finite (albeit an incredibly small value) for any x. Thus, difference on tails can be expected -see Fig. 20.

Project Think how this can be cured and construct a better approximation.

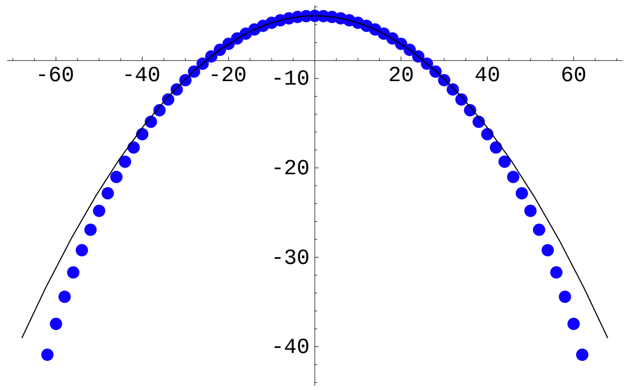

FIG. 20: Non-biased random walk and the diffusion approximation on a log scale

Dr. Vitaly A. Shneidman, Phys/MtSE 788, 8th Lecture

XIV. DIFFUSION IN FREE SPACE FOR $D = 1, 2, 3$

will be discussed in class.

$$G[r,t] = \frac{1}{\{4\pi t\}^{d/2}} \exp\left[-\frac{r^2}{4t}\right]$$

(the Green's function for any $d = 1, 2, 3$)

Normalization:

$$\int d^d r G[r,t] = 1$$

with $d^2r = 2\pi r dr$ and $d^3r = 4\pi r^2 dr$ (HW: verify the above and verify that G satisfies the diffusion equation for any d)

Constant source:

$$\int_0^\infty G[r,t]dt = \frac{1}{4}\pi^{-d/2} r^{2-d} \Gamma[d/2-1] \, , \quad d > 2$$

No steady-state for $d \leq 2(!)$

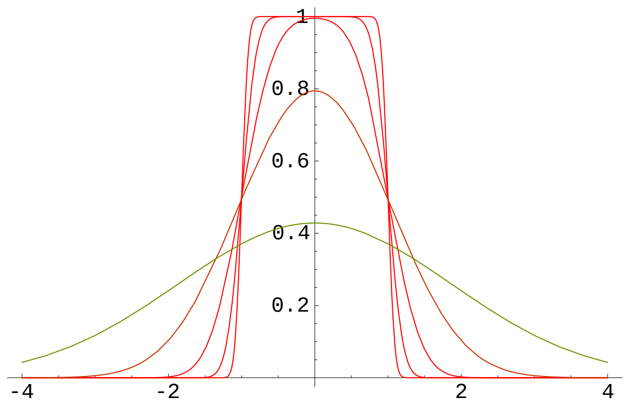

FIG. 21: Diffusion of an initially constant distribution in free space

XV. THE DIFFUSION EQUATION IN 1 D

A. Free boundaries

General solution (1d):

$$c(x,t) = \int_{-\infty}^{\infty} dy G[x-y,t] c_0(y)$$

the above is general for initial distribution c_0; below is an example of a localized intial distribution between $x = 0$ and $-\infty$:

$$c_{an}[x,t] := \frac{1}{2}\mathrm{erfc}\left[\frac{x}{2\sqrt{t}}\right]$$

(see diffusion2.nb)

Another example: $c_0 = 1$ for $0 < x < 1$. From superposition principle:

$$c_{box}[x,t] = (c_{an}[x-1,t] - c_{an}[x+1,t])/2$$

B. Problems with boundaries

1. *Semi-infinite: fixed concentration*

$$c(0,t) \equiv 1$$
$$c(x,t) = 2c_{an}[x,t] = \mathrm{erfc}\left[\frac{x}{2\sqrt{t}}\right]$$

guessed !! (yes, guessing is legal!); same figure as before, only now the region $x < 0$ is "unphysical"

2. *Semi-infinite: reflecting*

point source at $x = 1$ and reflecting boundary at $x = 0$. $j = 0$, thus $\partial c/\partial x = 0$ at the reflecting boundary.

$$c_{mir}[x, t] := G[x - 1, t] + G[x + 1, t]$$

3. *semi-infinite: absorbing*

Absorbing boundary at $x = 0$ and point source at $x = 1$.

$$c_{abs}[x, t] := G[x - 1, t] - G[x + 1, t]$$

Note : do not care about negative concentration at $x < 0$

C. Two absorbing boundaries: Fourier expansion

1. *Formulation of the problem*

A. Solve the equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{62}$$

in the interval

$$0 \leq x \leq l$$

with $l = 1cm$, $D = 10^{-8}m^2/s$ and the boundary conditions (BC)

$$c(0, t) = c(l, t) = 0$$

The initial condition is

$$c(x, 0) = f(x)$$

Select any simple function $f(x)$ (e.g., a linear function $f(x) = ax + b$, or a boxed function f(x)=1 for $l/2 - h/2 \leq x \leq l2 + h/2$ - Appendix A for *Mathematica* hints).

B. Plot graphs for concentrations at different points for $t = 1h,\ t = 2h,\ t = 4h,\ t = 6h$ and compare analytical and numerical results.

Start: Dimensionalization: Switch to new time

$$t' = Dt/l^2$$

so that

$$\frac{\partial c}{\partial t'} = \frac{\partial^2 c}{\partial x^2} \tag{63}$$

In that form the equation is ready to be passed to a mathematician (we do not scale x since l is 1cm).

2. Analytical solution

Below the method of separation of variables is applied; other methods (Laplace transform, reflection etc.) also can be used. Primes will not be indicated further in eq.(75).

We look for a solution

$$c(x,t) = \sum_{n=1}^{\infty} A_n \exp\left(-\lambda_n^2 t\right) \sin(n\pi x) \tag{64}$$

[Note: In each term of the sum the x- and t-dependencies are separated. A simple exponential dependence on t is expected since there is only a first derivative in t and coefficients are t-independent. The function $\sin(n\pi x)$ for integer $n = 1, 2, 3...$ satisfies the diffusion equation (75) and the BC.]

Substituting the above expansion in eq.(75) and comparing coefficients at each $\sin(n\pi x)$, one obtains:

$$\lambda_n^2 = \pi^2 n^2$$

for the eigenvalues. To obtain the expansion coefficients, A_n, we note that

$$\int_0^1 \sin(n\pi x)\sin(m\pi x)dx = 0$$

for $m \neq n$ and equals 1/2 for $m = n$. Then, we consider eq.(64) at $t = 0$ with $c(x, 0) = f(x)$. Multiplying the expansion by $\sin(m\pi x)$ and integrating from 0 to 1, one obtains

$$\int_0^1 dx f(x)\sin(n\pi x) = \frac{1}{2}A_n \tag{65}$$

For simple $f(x)$ the integral can be evaluated analytically (e.g, with *Mathematica* help). After this, the expansion (64) gives the full analytical solution. If the time is not too small, the solution is accurately approximated by the first few terms. It can be plotted easily using any program; *Mathematica* is one of the possibilities.

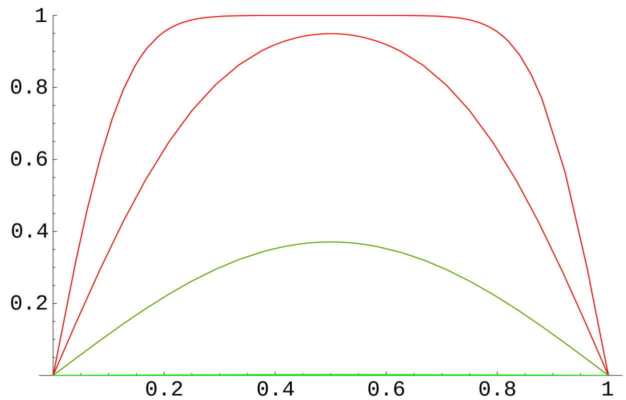

FIG. 22: Diffusion of an initially constant distribution between two absorbing boundaries

D. Numerical

Let us break the x-interval into N segments with $\delta x = 1/N$. There is now an array of $N+1$ concentrations $c_j(t)$ with $j = 0, 1, 2, ..., N$ and with $c_0 = c_N = 0$. The simplest method is to replace the second derivative in eq.(75) by the second difference:

$$\left.\frac{\partial^2 c}{\partial x^2}\right|_{x=x_j} \to \left[c_{j+1} + c_{j-1} - 2c_j\right]/(\delta x)^2$$

where $x_j = j \cdot \delta x$ is the discrete coordinate.

Thus one gets a system of ordinary differential equations

$$\frac{dc_j}{dt} = \left[c_{j+1} + c_{j-1} - 2c_j\right]/(\delta x)^2 \ , \ \ 1 \leq j \leq N-1 \tag{66}$$

with initial conditions

$$c_j(0) = f(x_j)$$

Various ways to solve the resulting equations wil be discussed later in the course.

E. Laplace Transform

The same problem. See the Mathematica notebook. After switching to the LT, the diffusion equation becomes an *ordinary* differential equation, and can be solved in elementary functions. Further, we expand the denominator assuming large s to emphasize the role of small t (and to simplify inversion). One obtains

$$W[x,s] = \frac{1 + e^{-\sqrt{s}} - e^{-\sqrt{s}x} - e^{-\sqrt{s}(1-x)}}{s} \sum_{m=0}^{\infty} (-1)^m e^{-m\sqrt{s}}$$

Inverse of

$$e^{-\sqrt{s}(x+m)}/s$$

is

$$i_m[x,t] \equiv \operatorname{erfc}\left[\frac{m+x}{2\sqrt{t}}\right]$$

Thus,

$$c[x,t] = \sum_{m=0}^{\infty} (i_m[0,t] + i_m[1,t] - i_m[x,t] - i_m[1-x,t])$$

For a given accuracy, $\epsilon \ll 1$ one has an estimation

$$m \sim 2\sqrt{t}\ln(1/\epsilon)$$

which is a modes number (for a computer) for not too large t. With such a cut-off on m evaluation of the sum (and plotting) are fast on any platform.

XVI. PROJECT 1

- describe in detail the full solution of the 1-dimensional problem with 2 absorbing boundaries, using both Fourier and Laplace
- estimate the minimal number of terms in each expansion to reach a given accuracy (say, 10^{-16})
- make a single expression which would automatically select the expansion with less terms (depending on time)
- make a good plot
- Extra: consider a different, say linear, initial distribution

XVII. HIGHER DIMENSIONS. STEADY-STATE

$$\Delta c = 0$$

A. $d = 1$

Consider boundary conditions $c(0,t) = c_0$, $c(l,t) = 0$ which lead to steady-state concentration

$$c = ax + b = c_0(1 - x/l)$$

(cannot take $l \to \infty$).
Flux

$$j = Dc_0/l = const$$

(typical for 1d)

B. $d = 2$

Two coaxial cylinders, $c(a) = c_0$, $c(b) = 0$

$$(rc')' = 0$$

$$c = A + B \ln r = c_0 \frac{\ln(b/r)}{\ln(b/a)}$$

Again, need boundaries: cannot take $a \to 0$ or $b \to \infty$. Can consider, however,

$$a \to 0 \ , \quad c_0/\ln(1/a) = const$$

Flux:

$$j(r) = Dc_0 \frac{1}{r \ln(b/a)}$$

Total flux:

$$J = 2\pi r j = 2\pi D c_0 \frac{1}{\ln(b/a)} = const$$

HW: *consider evaporative BC*

$$dc/dr + h\,(c - c_{eq}) = 0$$

find flux and study it as a function of b/a

C. $d = 3$

Two concentric spheres, $c(a) = c_0$, $c(b) = 0$

$$\left(r^2 c'\right)' = 0$$

$$C = B + A/r = c_0 \frac{a(b-r)}{r(b-a)}$$

For $b \to \infty$

$$c = ac_0/r$$

(no problem).

XVIII. TIME-DEPENDENT, $d = 2$

Diffusin with $D = 1$ inside a cylinder with $R = 1$, $c(R,t) \equiv c_0$, $c(r,0) = 0$.

New variable to get zero BC:

$$f(r,t) = c(r,t) - c_0 \ , \quad f(r,0 = -c_0$$

XIX. SEPARATION OF VARIABLES

Look for

$$u(r) \exp\left(-\lambda^2 t\right)$$

with

$$\frac{1}{r}\left(ru'\right)' + \lambda^2 u = 0 \tag{67}$$

with solution

$$J_0(\lambda r)$$

(the other solution is infinite at $r = 0$). From the BC:

$$J_0\left(\lambda\right) = 0$$

i.e. $\lambda = \lambda_n$, the n-th root of J_0.

Thus,

$$f(r,t) = \sum_{n=1}^{\infty} b_n J_0\left(\lambda_n r\right) e^{-\lambda_n^2 t}$$

with

$$f(r,0)=\sum_{n=1}^{\infty} b_n J_0\left(\lambda_n r\right)$$

Using

$$\int_0^1 rJ_0\left(\lambda_n r\right) J_0\left(\lambda_m r\right) dr = 0\ , \quad m\neq n$$

and

$$\int_0^1 rJ_0^2\left(\lambda_n r\right) dr = \frac{1}{2} J_1^2\left(\lambda_n\right)$$

one obtains b_n (see below).

HW check the above identities

$$b_n\int_0^1 f(r,0)J_0^2\left(\lambda_n r\right) rdr = -\int_0^1 J_0^2\left(\lambda_n r\right) rdr = -J_1\left(\lambda_n r\right)/\lambda_n$$

(HW - check the last relation from books or Mathematica) Thus,

$$b_n = \frac{2}{\lambda_n J_1\left(\lambda_n\right)}$$

see the *Mathematica* handout with graphics and the Bessel package.

A. Small time: Laplace

Equation for LT is similar to the one which follows from separation of variables but with $-s$ instead of λ^2. Thus, modified Bessel. With $c_0=1$, solution

$$C(r,s)=\frac{I_0\left(r\sqrt{s}\right)}{sI_0\left(\sqrt{s}\right)}$$

Expanding for $s\to\infty$, one gets an expansion in terms of

$$\mathrm{i^n erfc}\left(\frac{x}{2\sqrt{t}}\right)$$

(see Mathematica handout). The 1st term,

$$\mathrm{erfc}\left(\frac{x}{2\sqrt{t}}\right)$$

is similar to the flat case.

XX. PROJECT : AN APPLIED PROBLEM WITH NON-LINEAR BOUNDARY CONDITIONS FOR THE DIFFUSION EQUATION

A. Introduction

This research project is part of the Phys 788/MtSE 788 course. The goal is to introduce students to a delicate interplay of analytics and numerics when studying a close-to-life applied problem.

The problem is from the book by P. Shewmon "*Diffusion in Solids*", but with variable parameters and with additional tasks.

B. Formulation of the problem

Hydrogen at 1 MPa is to be stored at 400^o C in outer space, in a spherical iron tank with an inner radius a and an outer radius b. You are a) to calculate the rate of pressure drop (MPa/s) as a result of diffusion of hydrogen through the wall and b) to calculate the relative concentration of hydrogen in iron (in gmH/gmFe) as a function of time.

Take the diffusion coefficient $D = 10^{-8}$ m^2/s, and assume that the concentration of hydrogen in the iron at either side of the wall is the equilibrium solubility given by the equation

$$C(P) = 10^{-5}\,(p)^{1/2}\ \ gmH/gmFe \quad (P \text{ in MPa}) \tag{68}$$

Plot results for $a = .1$m and $b = 0.101$m, $b = 0.2$m, $b = \infty$.

Extra credit. The same problem, but for a long cylindrical tank.

C. Mathematical formulation

D. Diffusion in iron

One has for the concentration $c\,(\vec{r},\ t)$

$$\frac{\partial c\,(\vec{r},\ t)}{\partial t} = D\nabla^2 c\,(\vec{r},\ t) \tag{69}$$

Since the problem is spherically symmetric, one has

$$\frac{\partial c(r,t)}{\partial t} = D\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}c(r,t)\right) \tag{70}$$

The boundary conditions to this equation are given by eq.(68).

E. Pressure Drop

Pressure drop results from leakage of hydrogen into iron. The flux density of hydrogen inside iron (at any r) is given by

$$j(r,t) = -D\partial c(r,t)/\partial r$$

Thus, the full flux into iron is given by

$$I(t) = 4\pi a^2 j(a,t) = -\ 4\pi a^2 D \left.\frac{\partial c(r,t)}{\partial r}\right|_{r=a} \tag{71}$$

If the dimension of c (for the moment at least) is # of molecules per m^3, then the rate at which molecules are lost from the gas is given by

$$\frac{dN}{dt} = -I \tag{72}$$

The ideal gas law

$$P = N/(4/3\ \pi a^3) \cdot kT$$

(T being absolute temperature and k Boltzmann constant) relates N to pressure; a factor 10^{-6} should be introduced if P is in MPa, and all the rest in SI units.

If concentration c is *relative* to iron, eq.(71) is to be multiplied by n_{Fe}, the concentration of Fe atoms. Further, as usual for the diffusion problem, we will use a
new "time" = "old time" $\cdot$ D.
(No new notations will be used, but the final time should be divided by D if one wants to get it in seconds). Similarly, to we will use a concentration multiplied by 10^5 in order to get rid of a small factor in boundary conditions; again we will still use c, but the final answer should be reduced by 10^5 to get gmH/gmFe.

One thus has

$$\frac{dP}{dt}\ \text{(in MPa/s)}\ = \frac{\alpha}{a} \left.\frac{\partial c(r,t)}{\partial r}\right|_{r=a} \tag{73}$$

with

$$\alpha = 3 \cdot 10^{-11} k n_{Fe} T \tag{74}$$

and

$$\frac{\partial c(r,t)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}c(r,t)\right) \tag{75}$$

(**Task 1.** Calculate the number for α at the given temperature.)

Equations (73) and (75) together with the initial condition $P(0) = 1$ and the boundary conditions

$$c(a) = \sqrt{P}\ ,\quad c(b) = \sqrt{P_{atm}} \tag{76}$$

give a full description of the problem. Note that P_{atm} is the partial pressure of hydrogen in atmosphere in MPa.

(**Task 2.** Find out the value of P_{atm}.)

F. Overview

We succeeded in casting the equations in a form convenient for mathematical study. There is now a single parameter α which (together with a and b) determines the solution.

The system of equations (73, 75,76) cannot be solved exactly due to the non-linear boundary condition, eq.(76). We can thus choose two ways. The first is a reasonable analytical approximation. The second is a full numerical solution of the problem.

What is the reason to expect an accurate analytical approximation? - It is is the small value of α. Note that for $\alpha = 0$ the pressure and concentration equations become decoupled from each other. Here the diffusion equation can be solved exactly, approaching a steady state. For non-zero but small α one can expect that concentration still remains close to steady state, but with a factor which slowly drifts with time. This is called "quasi-steady-state". Accuracy of the approximation will depend on whether indeed the time to establish steady-state inside the iron is smaller than the characteristic time scale of pressure drop. Intuitively, this will happen for reasonably thin walls (a more precise criterion can be established *a posteriori*). The quasi-steady-state approximation will not work for $b \to \infty$ (cavity with hydrogen in bulk iron) when describing concentration, but still can work to determine dP/dt.

G. Analytics: Quasi-steady-state

1. *The thin-wall approximation*

Consider

$$d \equiv b - a \ll a \ ,$$

a "thin wall". There is not much difference now from a flat membrane. The gradient of concentration is approximately constant given by

$$dc/dr \approx -\left[c(a) - c(b)\right]/d$$

Neglecting $c(b)$ and using the condition (73) one obtains

$$\frac{dP}{dt} = -\frac{\alpha}{ad}\sqrt{P}$$

which gives

$$\sqrt{P(t)} = \sqrt{P(0)} - \frac{\alpha t}{2ad}$$

(**Task 3**. Find $P(t)$ not neglecting P_{atm}. Compare with above).

2. *Thick wall*

Using a substitution

$$c(r,t) = \chi(r,t)/r$$

the spherically symmetric diffusion equation is reduced to a one-dimensional form

$$\frac{\partial \chi}{\partial t} = \frac{\partial^2 \chi}{\partial r^2} \tag{77}$$

(Note: there is no similar simple trick for cylindrical problem!)

We are interested in steady-state with

$$\chi(r) = A + Br$$

A and B are determined by boundary conditions. E.g., for an infinite wall one should have $B = 0$ and $A = ac(a)$. Thus,

$$c_\infty(r) = c(a)a/r$$

and one has

$$\frac{dP}{dt} = -\frac{\alpha}{a^2}\sqrt{P}$$

The rest is similar to the thin-wall case.

(**Task 5**. Do the general case, $b < \infty$). Plot graphs and compare.

(**Task 6**. Try to establish the limits of applicability of the quasi-steady-state approximation; the thin-wall case is the simplest).

H. Numerical

Since eq. (77) looks 1-dimensional, we use the same ideas as described before project 1. The interval between a and b is broken into a large number (M) of small intervals with width

$$\delta = (b - a)/M$$

This gives a set of *ordinary* differential equations for χ_1, χ_2, etc., which can be solved using standard approaches. There is a difference in boundary conditions

$$\chi_0(t) = a\sqrt{P(t)}$$

with an extra differential equation

$$\frac{dP}{dt} = \frac{\alpha}{a^2}\left\{\frac{d\chi}{dr} - \frac{\chi}{r}\right\}$$

(**Task 7**. Re-write the above in terms of discrete χ_0, χ_1. Write a full system of equations you will be solving).

(**Task 8**. Write a program (any language), compare with analytics).

XXI. VARIABLE $D = D(c)$

Consider 1-d and steady state with

$$D = D_0 \left[1 + f(c)\right]$$

In steady-state

$$-D\frac{dc}{dx} = j = const = J$$

Thus,

$$\int D(c)dc = -Jx + B$$

or with

$$F(c) \equiv \int_0^c f\left(c'\right) dc'$$

$$D_0 \left[c + F(c)\right] = -Jx + B \tag{78}$$

Let

$$c(0) = c_0\ ,\quad c(l) = 0$$

From BC at $x = 0$:

$$B = D_0 \left[c_0 + F\left(c_0\right)\right]$$

the other BC:

$$-Jl + B = 0$$

Thus from eq. (78)

$$\frac{c - c_0 + F(c) - F\left(c_0\right)}{c_0 + F\left(c_0\right)} = -\frac{x}{l} \tag{79}$$

Example: $f(c) = ac/c_0$, $[a] = 1$, $F(c) = (1/2)ac^2$. With $y = x/l$ and $z = c/c_0$

$$\frac{z - 1 + 1/2 \cdot az^2}{1 + a/2} = -y$$

(see the *Mathematica* printout with plots).

HW - explore the limits of a. For $a = 1$ find numerically $c(x)$ and make a few plots $c(x)$.

XXII. NUMERICAL SOLUTIONS

we consider a one-dimensional equation with $D = 1$

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

(D will be re-introduced into some of the results for clarity).

A. Discretization in space. Exponential solution.

$$\left.\frac{\partial^2 c}{\partial x^2}\right|_{x=x_j} \to \left[c_{j+1} + c_{j-1} - 2c_j\right]/(\delta x)^2$$

where $x_j = j \cdot \delta x$ is the discrete coordinate and the dimension is N.

Thus one gets a system of ODE's

$$\frac{dc_j}{dt} = \left[c_{j+1} + c_{j-1} - 2c_j\right]/(\delta x)^2 \tag{80}$$

If we introduce a matrix $\hat{m}$ with

$$m_{ik} = -1\ (i = k)\ ,\quad m_{ik} = \frac{1}{2}\ (i = k \pm 1)\ ,\quad m_{ik} = 0\ \text{ otherwise}$$

and an N-dimensional vector $\vec{c} = (c_1\ ,\ c_2\ ,\ \ldots)$ then

$$\frac{d\vec{c}}{dt} = \frac{2}{\delta x^2}\hat{m} \cdot \vec{c}$$

The formal solution is

$$\vec{c}_{exp}(t) = \exp\left\{\frac{2t}{\delta x^2}\hat{m}\right\} \cdot \vec{c}(0)$$

Since *Mathematica* "knows" the exponential of a matrix, it is possible to test this against the Green's function of the exact diffusion equation - see 788_diff4.nb with *mat1* corresponding to $\hat{m}$ and v to c. In practice, however, there is too much strain on computer if N (*dim* in 788_diff4.nb) is large.

B. Discretization in t

Let dt be the discrete step in time. Then

$$\vec{c}(t + dt) = \vec{c}(t) + \frac{2dt}{\delta x^2}\hat{m} \cdot \vec{c} \tag{81}$$

or with $\hat{I}$ being the identity matrix,

$$\vec{c}(t+dt) = \hat{M}_r \cdot \vec{c}(t)\ ,\quad \hat{M}_r = \hat{I} + 2r\hat{m}\ ,\quad r \equiv \frac{dt}{\delta x^2} \tag{82}$$

If n steps in time are made,

$$\vec{c}_{pow}\left(ndt\right) = \hat{M}_r^n \cdot \vec{c}(0) \tag{83}$$

(note that exponential solution appears for $r \to 0$).

The solution is accurate and fast, but becomes unstable for larger dt. Why? Note the the problem is identical to random walk with r being the probability to step right or left. Then, $1-2r$ is the probability to stay, or

$$r \equiv \frac{D\ dt}{\delta x^2} \le \frac{1}{2} \tag{84}$$

One can test that absolute values of some eigenvalues of $\hat{M}_r$ are larger than 1 for $r > 1/2$ (see 788_diff4.nb). More formally, criteria of stability are established by the von Neumann stability analysis:

C. von Neumann stability analysis

Ignore the boundaries, etc. Look for

$$v\left(j\delta x, t\right) \sim e^{ikj}e^{\lambda t}$$

one gets

$$e^{\lambda} = 1 + 2r(\cos(k) - 1) = 1 - 4r\sin^2(k/2)$$

If any k, then for $r > 1/2$ one has $e^{\lambda} < -1$ (λ complex). Thus,

$$e^{\lambda} \times e^{\lambda} \times e^{\lambda} \ldots - \text{diverges!}$$

D. Backward (implicit) scheme

Instead of eq. (81)

$$\vec{c}(t+dt) = \vec{c}(t) + \frac{2dt}{\delta x^2}\hat{m} \cdot \vec{c}(t+dt) \tag{85}$$

or

$$\vec{c}(t) = \hat{M}_{-r} \cdot \vec{c}(t+dt)$$

Thus,

$$\vec{c}(t+dt) = \left(\hat{M}_{-r}\right)^{-1} \cdot \vec{c}(t)$$

This is stable - see 788_diff4.nb. Or, von Newmann analysis:

$$e^{\lambda} = 1 - e^{\lambda} 4r \sin^2(k/2)$$

with

$$e^{\lambda} = \frac{1}{1 + 4r \sin^2(k/2)}$$

Thus, for any $r > 0$

$$\left|e^{\lambda}\right| < 1$$

(yes!)

Alternative - Crank-Nicholson.

XXIII. LAPLACE EQUATION IN A SEMI-INFINITE STRIPE

Consider the following 2D problem:
two parallel conducting planes are separated by a distance $a = 1$ in the x-direction and are at zero potential. Between the planes there is a semi-infinite conducting slab with thickness $a - 0$ which down extends from $y = 0$ and which is at potential V. Find the distribution of potential in the stripe $0 < x < a$ and $0 < y < \infty$.

This is a rich problem which will allow us to

- consider the solution via separation of variables
- examin singularities near the corners and discuss the dimensional analysis
- briefly consider relation to the theory of analytic functions (complex variables) where the problem does have a closed solution (though, lets forget about it for the moment
- introduce numerical methods of solving the Laplace equation

A. Separation of variables

Since we have rectangular geometry, natural to consider Cartesian coordinates. Look for a solution

$$V(x,y) = \sum_k a_k X_k(x) Y_k(y) \tag{86}$$

(can do this because the Laplace equation is linear). Consider now a term in the above sum (drop the k-index for the moment)

$$\hat{\Delta}\left(X(x)Y(y)\right) = Y\frac{d^2X}{dx^2} + X\frac{d^2Y}{dy^2} = 0$$

or

$$\frac{1}{X}\frac{d^2X}{dx^2} = -\frac{1}{Y}\frac{d^2Y}{dy^2} = -\lambda^2 \tag{87}$$

Now

$$Y(y) \propto e^{-\lambda y}$$

thus $\lambda > 0$. Next,

$$X(x) \propto \sin(\lambda x)$$

and from $X(1) = 0$

$$\lambda_n = n\pi \ , \quad n = 1, 2, \ldots$$

To get coefficients in eq. (86) consider $y = 0$:

$$V = \sum_n a_n \sin(\lambda_n x)$$

multiply by $\sin(\lambda_m x)$ and integrate. From orthogonality (HW - check!)

$$a_n = 2V \int_0^1 \sin(n\pi x) dx$$

which is $4V/(\pi n)$ for n odd and 0 for n even (HW - check). Thus,

$$V(x, y) = \frac{4V}{\pi} \sum_{k=0}^{\infty} \frac{1}{2k+1} \exp\{-(2k+1)\pi y\} \sin\{(2k+1)\pi x\} \tag{88}$$

This is a formally exact solution. In practice need to know, how many terms contribute? The extereme is $k = 0$ with

$$V(x, y) \simeq \frac{4V}{\pi} \exp\{-\pi y\} \sin\{\pi x\} \quad y \to \infty$$

More general, suppose we fix the desired relative accuracy, ϵ. Then,

$$n \sim \frac{\ln(1/\epsilon)}{\pi y}$$

this is weakly sensitive to ϵ, and because of π gives a small n for finite y. Thus, for $y \gtrsim 1$ the leading asymptote is an excellent approximation. But what about $y \to 0$? Need an *infinite* number of terms! Any program, including *Mathematica*, will fail. What to do? Rearrange!

$$V(x, y) = V + \frac{4V}{\pi} \sum_k \frac{1}{2k+1} \left[\exp\{-(2k+1)\pi y\} - 1\right] \sin\{(2k+1)\pi x\} \tag{89}$$

(HW - check that the part of the sum with -1 indeed cancels V). With just a few k this should give a good approximation for small y.

HW: *write a Fourier series if the stripe is replaced by a finite rectangle with the same zero potential on the upper side as on the vertical sides. Explore the limits of a "tall" and "short" rectangle.*

B. Edge

Expand eq. (88) to obtain

$$V(x,y) \simeq V - 4Vy \sum_k \sin\{(2k+1)\pi x\} \tag{90}$$

After summation:

$$V(x,y) \simeq V\left[1 - \frac{2y}{\sin(\pi x)}\right] \ , \quad y \to 0 \tag{91}$$

HW: *check this (Mathematica is fine)*

C. Corner

Hard to get from a series; better start again:

$$\Delta V = 0$$

Look for $V = V(r,\theta)$, but no length scale!!!. Thus,

$$V = V(\theta)$$

Now use

$$\Delta V(\theta) = \frac{1}{r^2}\frac{d^2V}{d\theta^2} = 0$$

or (with BC)

$$V(\theta) = \frac{2V}{\pi}\left(\frac{\pi}{2} - \theta\right)$$

In cartesian coordinates (since we use them elsewhere)

$$V(x,y) \sim \frac{2V}{\pi}\left(\frac{\pi}{2} - \arctan\frac{y}{x}\right) = \frac{2V}{\pi}\arctan\frac{x}{y} \tag{92}$$

For small x this is consistent with the edge expression, which is valid however only for $x \gg y$.

D. Relaxation method

In class. See 788_relax.pdf .

E. Project: Relation to complex variables - 2D only!

This is not in Jackson, but allows to solve his problem analytically

1. Cauchy-Riemann conditions

If

$$f(z) = u(x, y) + i\, v(x, y) \tag{93}$$

then for the limit

$$\lim_{\Delta\, z \to 0} \frac{f\,(z + \Delta\, z) - f(z)}{\Delta\, z}$$

to be independent of the direction of $\Delta\, z$:

$$\frac{\partial}{\partial x} u = \frac{\partial}{\partial y} v\ , \quad \frac{\partial}{\partial y} u = -\frac{\partial}{\partial x} v \tag{94}$$

Thus,

$$\Delta u = \Delta v = 0 \tag{95}$$

2. Complex potential

We used

$$\hat{\nabla} \times \vec{E} = 0$$

to introduce $\vec{V} = -\hat{\nabla}\Phi$. Another condition (with no charges)

$$\hat{\nabla} \cdot \vec{E} = 0 \tag{96}$$

Thus, one can introduce $\vec{A}$ with

$$\vec{E} = \hat{\nabla} \times \vec{A} \tag{97}$$

(Note: In ch. 6 Jackson does something similar with magnetic field $\vec{B}$ -for which it is much more meaningful since $\hat{\nabla} \cdot B$ is *always* zero).

For a $3D$ space this $\vec{A}$ is not a big help, but if one has a $2D$ field $\vec{E}(x, y)$ one can select $\vec{A}(x, y)$ in the z-directions so that

$$E_x = \frac{\partial}{\partial y} A(x, y) = -\frac{\partial}{\partial x}\Phi(x, y)\ , \quad E_y = -\frac{\partial}{\partial x} A(x, y) = -\frac{\partial}{\partial y}\Phi(x, y)$$

Comapare this with Cauchy-Riemann! In other words,

$$\phi = \Phi - iA \tag{98}$$

is an *analytic* function of $z = x + iy$.

HW: *Construct $\vec{A}$ for a uninform field*

HW: *Show that $d\phi/dz = -E_x + iE_y$. Note that you can take the derivative in any convenient direction, e,g, x or y since w is analytic.*

Equation for a field line now reads

$$dx/E_x = dy/E_y$$

or

$$dx\frac{\partial}{\partial x}A(x,y) + dy\frac{\partial}{\partial y}A(x,y) \equiv dA = 0 \tag{99}$$

In other words elctric field lines correspond to $-Im[\phi] = const$ and are just as easy to plot as equipotential surfaces $Re[\phi] = const$.

HW: *Plot lines of $Re[\phi] = const$ and $-Im[\phi] = const$ for (a) $\phi = z$ and (b) $\phi = -\ln z$. To which electric fields they correspond?)*

READING: (optional) more general features are in Landau-Lifshits, vol.8, Ch. 1.3 and many practical examples of conformal mapping, both with and without electrostatic context, are in Kreyszig, Advanced Ehngineering Mathematics

3. Conformal mapping and solution of the problem

Returning to our problem we need the following:

- find a function $w(z)$ which mapps the stripe to a simpler shape with "good" boundary conditions (in our case it will be a right angle with potenatial V on one side and 0 on the other) - see Fig. 23.

- solve the problem, obtainig $\phi(w)$ (note: any analytical function $\phi(w)$ will satisfy the Laplace equation, but the proper one will also satisfy boundary conditions. (in our case we already solved the problem for the angle, so expect $\phi \propto \theta = -i\ln(w)$

- the function

  $$\phi\left(w(z)\right)$$

  will be the solution of the problem.

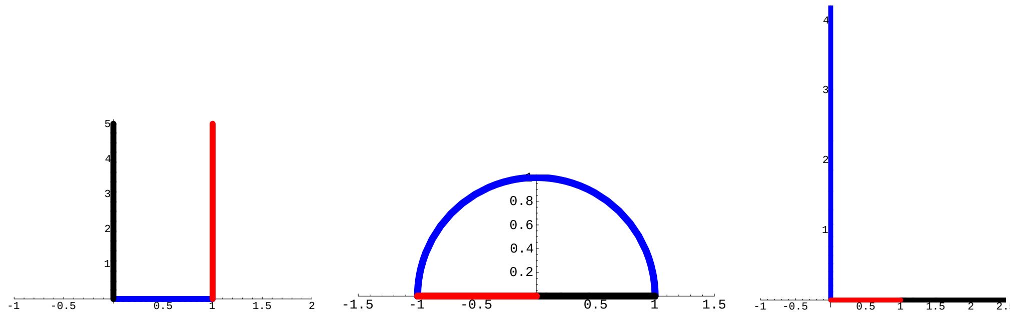

FIG. 23: Transformation from a semi-infite stripe in the z-plane to an angle in the w-plane via an intermediate semi-circle in the Z-plane. Colors track each side of the stripe. The functions are: $Z(z) = e^{i\pi z}$ and $w(Z) = (1+Z)/(1-Z)$. Direct conversion from stripe to corner is achieved by $w\left(Z(z)\right) = \left(1+\exp(i\pi z)\right) / \left(1-\exp(i\pi z)\right) = i\cot(\pi z/2)$ - see stripe.nb

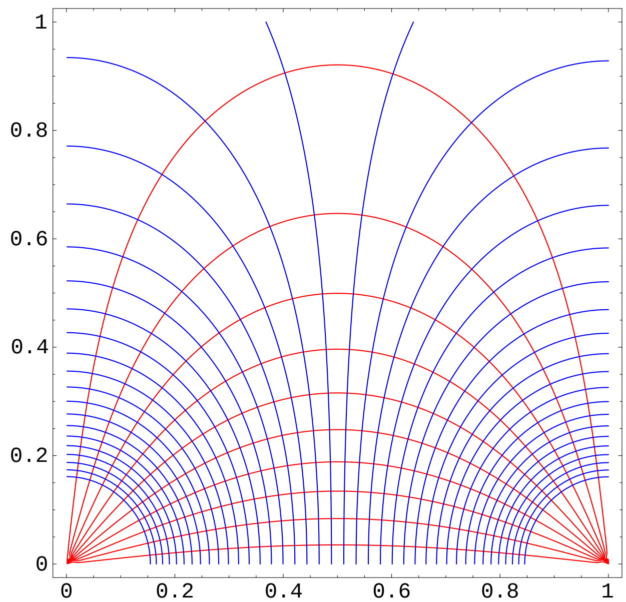

FIG. 24: Equipotential surfaces (red) and field lines (blue) for a stripe (semi-infinite in y-direction)

For the corner we have

$$\phi = -\frac{2V}{\pi} i \ln(w) \tag{100}$$

Thus, in original variables

$$\phi = -\frac{2V}{\pi} i \ln\left(i \cot\frac{\pi z}{2}\right) \tag{101}$$

which gives Fig. 24.

(THE REST WILL BE DISCUSSED IN CLASS)

XXIV. SCHRÖDINGER EQUATION

Steady-state: $\Psi = \Psi(\vec{r})$

$$-\frac{\hbar^2}{2m}\Delta\Psi + V\Psi = E\Psi \tag{102}$$

Several formulations:

- $E - V(\infty) > 0$ - scattering
- $E - V(\infty) < 0$ - eigenstates
- $V(\vec{r})$ periodic - bands

A. 1D - analytic

In 1D eq. (102) is ODE.

1. *Resonant levels*

Consider two δ-shaped barriers at $x = 0$ and $x = a = 1$ from each other. Outside of the barriers solutions are

$$\exp(\pm ikx)$$

with $k = \sqrt{2mE}/\hbar$. Barriers determine the discontinuity in 1st derivative.

Look for

$$\psi_1 = \exp(+ikx) + b\exp(-ikx)\ ,\quad x < 0$$

$$\psi_2 = c\exp(+ikx) + d\exp(-ikx)\ ,\quad 0 < x < a$$

$$\psi_3 = f\exp(+ikx)\ ,\quad x > a$$

For $a = 1$ and

$$\psi_1'(0) = -\omega\psi_1(0) + \psi_2'(0)$$

$$\psi_2'(1) = -\omega\psi_2(1) + \psi_3'(1)$$

one obtains an explicit solution. See Mathematica plot for $|f|^2$.

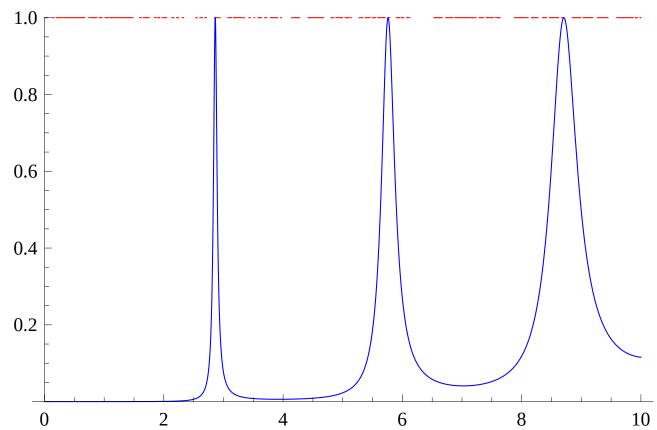

FIG. 25: Transmission coefficient $|f|^2$ through a pair of δ-barriers as a function of k (blue). Dimensionless "non-transparency" of a single barrier is $\omega = 20$. Red line is $|f|^2 + |b|^2 = 1$.

2. *Energy levels: WKB approximation*

$p(x)$ -classical

$$S \equiv \oint p dx = 2\pi\hbar \left(n + \gamma\right) \ , \quad n = 0, 1, 2, \ldots$$

γ - depends on BC; $\gamma = 1/2$ for smooth BC (follows from Airy function matching).

Mathematica realization:

1) calculate S for any energy

2) approximate $S(E)$ by a polynomial

3) solve for WKB condition (integer n), get E_n

(see the printout)

3. *Bands*

$$\psi\left(\vec{r}\right) = e^{i\vec{q}\vec{r}} u_{\vec{q}}\left(\vec{r}\right) \ , \quad u_{\vec{q}}\left(\vec{r} + \vec{a}\right) = u_{\vec{q}}\left(\vec{r}\right)$$

(Bloch, 1929).

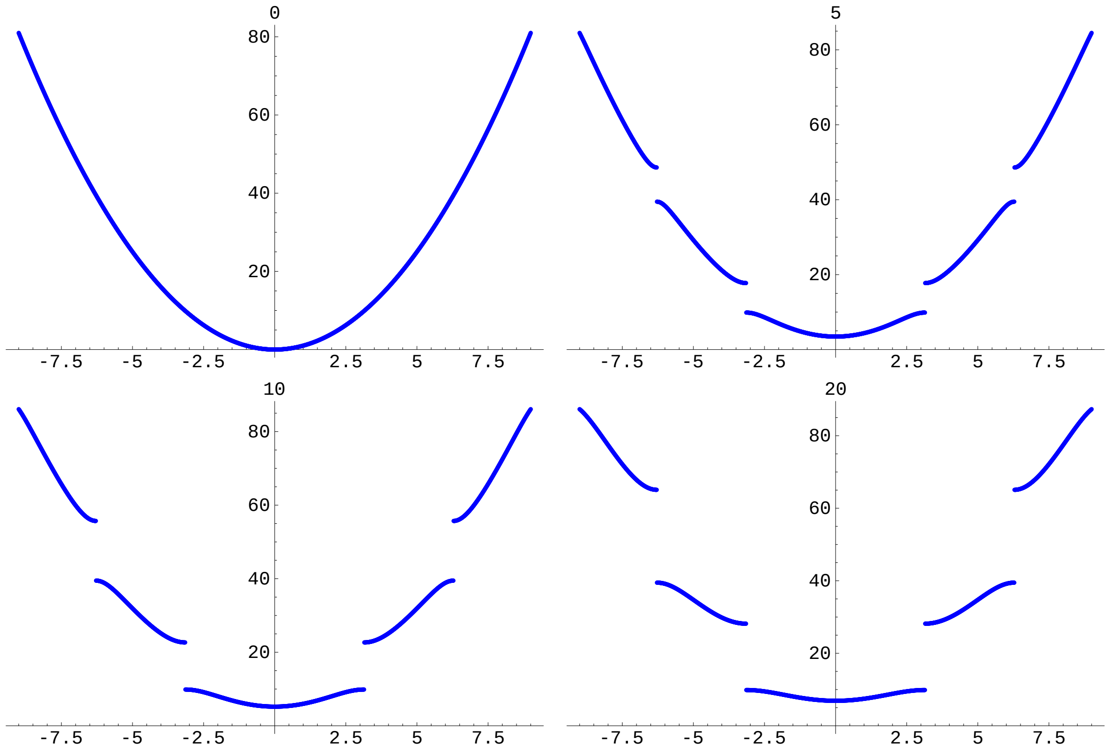

FIG. 26: Energy bands for the "Dirac comb" (Kronig-Penney model) for different values of the interaction potential.

B. Dirac comb

$$U(x) = \frac{\hbar^2}{m}\Omega \sum_{n=-\infty}^{\infty} \delta\left(x - na\right)$$

Let $a = 1$. Look for

$$\phi_1(x) = Ae^{ikx} + Be^{-ikx}$$

and

$$\phi_2(x) = e^{iq}\phi_1(x-1)$$

Have 2 conditions(BC) at $x = 1$, thus 2 homogeneous equations for A, B. Non-trivial solutions for

$$\cos q = \cos k + \omega \frac{\sin k}{k}$$

See Mathematica printout (Kronig.nb)

This determines bands in $\epsilon \equiv \hbar^2 k^2/2m$ as a function of q - see Fig. 26.

C. Numerical - matrix

Use discrete representation of d^2/dx^2. Construct a matrix *ham*, discrete analog of $\hat{H}$. Eigenvalues of this matrix are close to true eigenvalues. See the Mathematica printout for examples of harmonic potential and box.

Project: try to improve accuracy by using WKB BC; check for harmonic oscillator

D. Numerical - shooting

Idea: select a WKB BC (in "forbidden region $x \ll -1$"). For a selected E integrate the SE to get $\psi(x)$. For almost any E will have a diverging $\psi\left(x \to \infty\right) = \infty$. "Magic" E will correspond to small $\psi\left(x \to \infty\right)$.

Exremely accurate, if know where to look for. [If don't know -start from a WKB guess of E_n.

E. Numerics - variational

Key: select a good (intuitive!) trial function with several parameters. Then, the "average energy"

$$\int_{-\infty}^{\infty} \psi^* \hat{H} \psi dx$$

will have an extremum (min or max). This gives an equation for parameters, and will approximate the eigenfunction. The above integral will then approximate the energy.

We first try for a HO. A trial function

$$\exp\left(-ax^2\right)$$

will result in a correct $a = 1/2$. Then, we try a "bad" function for a box: instead of ısin, use polynomial.

For lowest level - usually extremely accurate. For higher levels a good guess is extremely important, otherwise many parameters.

F. Variational - 3D

Yukawa potential

$$U(r) = -\frac{1}{r}e^{-r/a}$$

see the *Mathematica* printout - file yukawa.nb

Project: Study the hydrogen atom; using the variational method and exact; compare

XXV. MONTE CARLO INTEGRATION

file *MonteCarlo.nb*

When to use?

- $d \geq 2$
- complicated (”bad”) boundary
- more-or-less smooth integrand (no peaks in small areas)
- not too high accuracy is ok

Note, sometimes you may have a ”good” boundary but a ”bad” integrand. If change of variables can reverse this, MC will work much better.

Ideas of MC - see Fig. 27. We want to find an area under the black arc (semicircle in this case) and to locate its center of gravity. Steps:

- surround by a simple boundary (blue box)
- define functions ”ar” (area) and ”mom” (moment) with zero initial value
- generate N points inside the box randomly
- if a points falls under the arc, increase ”ar” and ”mom” accordingly
- calculate averages ar/N, mom/N

Error decays as $1/\sqrt{N}$ - not too fast, but algorithm is very simple.

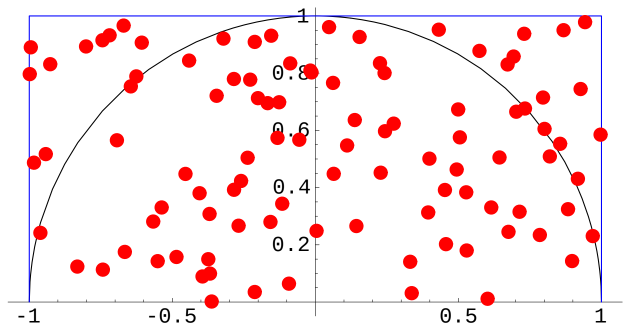

FIG. 27: Ideas of Monte Carlo integration

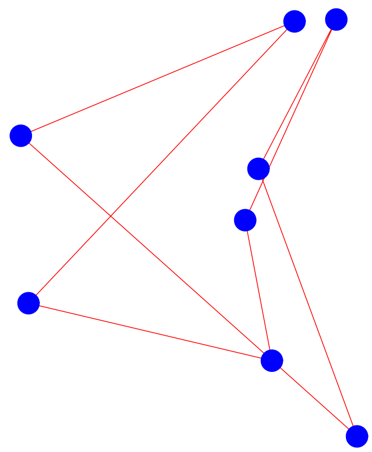

FIG. 28: An example of random path. Obviously, not the best.

XXVI. SIMULATED ANNEALING

$$prob(E) \propto \exp\left(-\frac{E}{k_B T}\right)$$

A. Travelling salesman problem

(will be discussed in class)

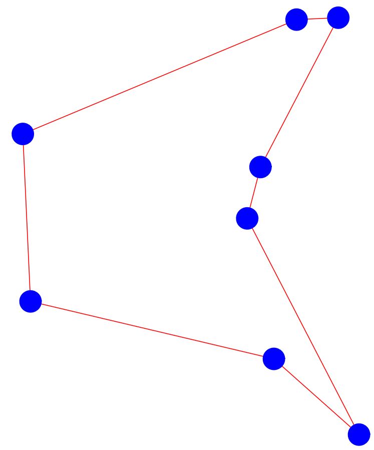

FIG. 29: The best path. Can be found exactly for $N \lesssim 10$, but otherwise one needs simulated annealing.

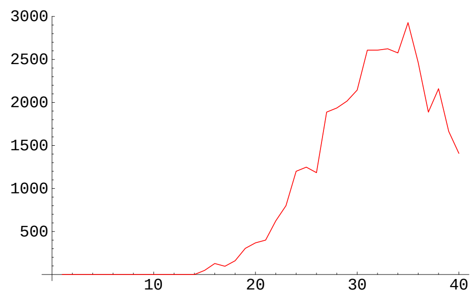

FIG. 30: Statistics of path lengths. Obviously, non-Gaussian.

XXVII. NON-EQUILIBRIUM ISING MODEL

A. Overview

1. Definitions

$$\mathcal{H} = -J \sum_{i,k}{}' s_i s_k - H \sum_i s_i \,, \quad s_i = \pm 1 \tag{103}$$

$J > 0$ - ferromagnet.

Equilibrium: $H = 0$. Model exactly solvable for square lattice ($\lambda = 4$), triagonal ($\lambda = 6$) and hexagonal ($\lambda = 3$), where λ is the number of nearest neighbors (NN).

$$t = 0: \quad s_i = -1\,, \quad 0 < H < \lambda \ \text{(metastability)}$$

2. Dynamics

Probability of a spin flip (*Glauber/Metropolis*):

$$P_{i \to f} = \frac{1}{\exp\left[\left(H_f - H_i\right)/k_b T\right] + 1} \ \text{ or } \ \frac{1}{\max\left\{\exp\left[\left(H_f - H_i\right)/k_b T\right],\, 1\right\}}$$

Alternative: Kawasaki dynamics (will not be used). Spin cannot flip but can exchange places with NN (diffusion).

3. Equivalence to a lattice gas

(Here we discuss square lattice only). Let only up-spins interact with each other (NN only) with "bond energy" ϕ. There is no interaction between up-down and down-down spins. Then treat down spins as background, individual up spins as "gas molecules" which can condense into a "liquid".

Input parameters are ϕ and μ. Gas and liquid are at equilibrium for "chemical potential"

$$\mu = \mu_0 = -2\phi$$

Otherwise gas will condense for $\mu > \mu_0$.

If

$$\phi = 4J$$

the thermodynamics of the equilibrium lattice gas and of the Ising ferromagnet will be the same. Furthermore, for "supersaturation"

$$S = \frac{\mu - \mu_0}{2\phi} \Longleftrightarrow \frac{H}{\phi} \tag{104}$$

the metastable behavior (and dynamics) will be equivalent as well.

B. Equilibrium (some analytics)

We use $k_B = 1$. Temperature is measured in units of J (i.e. $J = 1$).

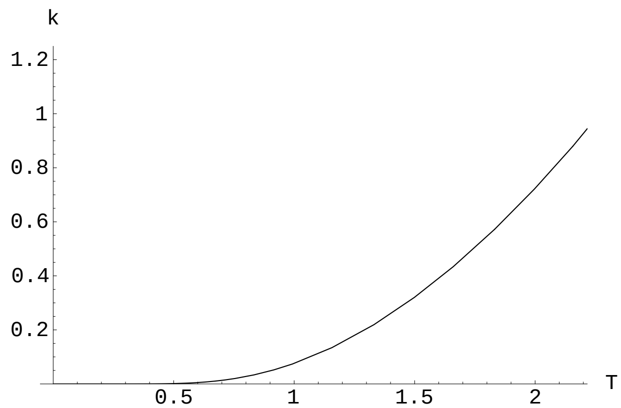

FIG. 31: The parameter $k(T)$. $k = 1$ corresponds to the critical temperature, T_c. Note that the curve is very flat at $T \lesssim 0.5$.

Main parameter (instead of temperature)

$$k(T) = \sinh(2/T)^{-2}$$

see Fig. 31. Critical temperature:

$$k(T_c) = 1$$

$$T_c = \frac{2}{\ln\left(\sqrt{2}+1\right)} = 2.26919...$$

HW: show or check this.

Free energy (per spin):

$$f(T) = -\frac{T}{2\pi}\int_0^\pi F(k,\theta)d\theta \tag{105}$$

with

$$F(T,\theta) = \ln\left\{2\left[1 + \frac{1}{k} + \frac{1}{k}\sqrt{1 + k^2 - 2k\cos 2\theta}\right]\right\}$$

Energy (per spin):

$$E = \frac{d(f/T)}{d(1/T)} = \frac{d(f/T)}{dk}\frac{dk}{d(1/T)}$$

Thus, with

$$e = \frac{\partial F(k,\theta)}{\partial k}$$

$$E = -\frac{dk}{d(1/T)}\frac{1}{2\pi}\int_0^\pi e(k,\theta)d\theta$$

From

$$f = E - Ts$$

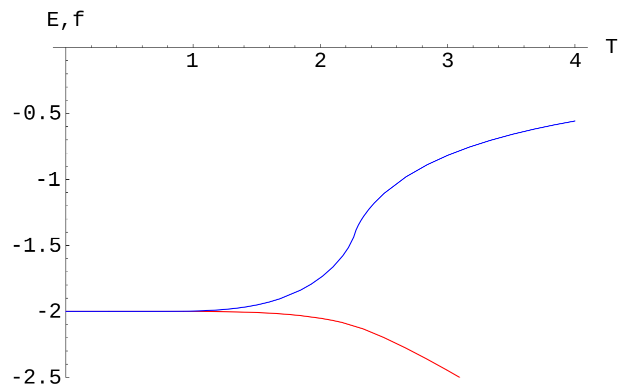

FIG. 32: Energy (blue) and free energy (red) per spin.

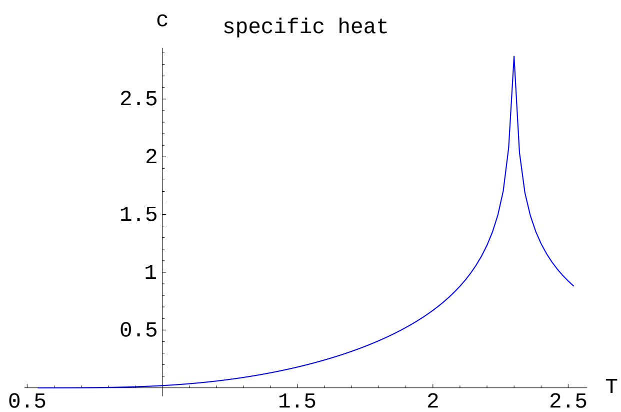

FIG. 33: "lambda point" of specific heat

energy and free energy should close at low temperature (small entropy), but E gets larger when T_c is approached -see Fig. 32.

Specific heat:

$$c_V = \frac{dE}{dT}$$

There is a "lambda-point" (logarithmic singularity) near T_c - see Fig. 33.

Magnetization:

$$m(T) = \left(1 - k^2\right)^{1/8}$$

Note a very small power (1/8) which makes the curve nearly vertical near T_c - see Fig. 34.

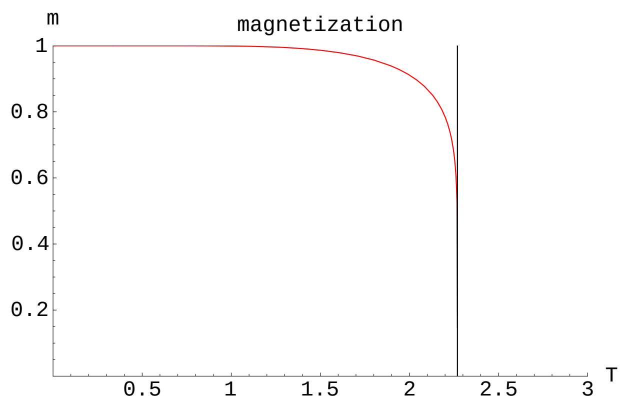

FIG. 34: Magnetization, $m(T)$. Note that $m(T) = 0$ for $T \geq T_C$ and that m is extremely close to 1 for $T \lesssim 0.5 T_C$

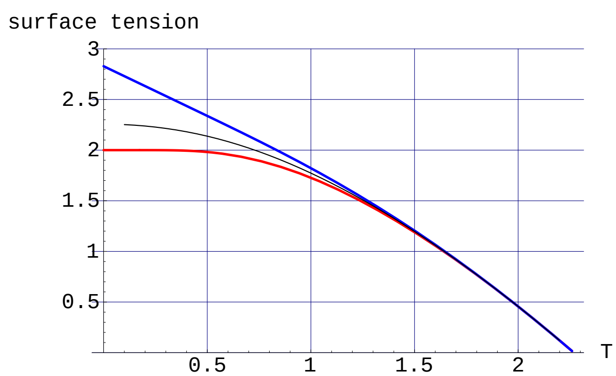

FIG. 35: The reduced interfacial tension σ in the directions parallel to the lattice (red) and diagonal (blue). The critical temperature is $T_c = 2.269\ldots$ (this corresponds to $J = 1$). Note that above $\sim 0.5\, T_c$ there is practically no anizotropy.

1. Interfacial tension

According to Onsager - see Fig. 37 :

$$\sigma_{||}/J = 2 + T/J \ln\left[\tanh(J/T)\right] \tag{106}$$

$$\sigma_{diag}/J = \sqrt{2}(T/J) \ln\left[\sinh(2J/T)\right] \tag{107}$$

With no anizotropy (higher $T < T_c$) a "droplet" will be practically round with radius R

$$\pi R^2 \simeq n$$

n - number of spins. The interfacial energy is given by

$$2\pi R\sigma_{eff} \tag{108}$$

where *any* of the two values of σ (parallel or diagonal) can be used for σ_{eff} .

At higher temperatures one can use the Wulff construction to find the shape of a droplet - this was done in early 80's by Rottman and Wortis and by Zia and Avron. The interfacial energy also can be calculated and used to define σ_{eff} . Form results of Zia and Avron one can obtain - see J. Chem.Phys., **111**, 6932 (1999)

$$\sigma_{eff} = \frac{2T}{\sqrt{\pi}}\sqrt{\int_{t_c}^{t} dt\ [1-q(t)] * \mathrm{K}\,[1-\mathrm{m}(t)]} \tag{109}$$

with $t \equiv 4J/T$, K - the elliptic integral, and

$$q(t) = \frac{3-e^{-t}}{\sinh t}\ ,\ \ \mathrm{m}(t) = 8\frac{\cosh t - 1}{(\cosh t + 1)^2} \tag{110}$$

This is shown by a black line in Fig. 37.

C. Non-equilibrium: simulations

Will be discussed in class.

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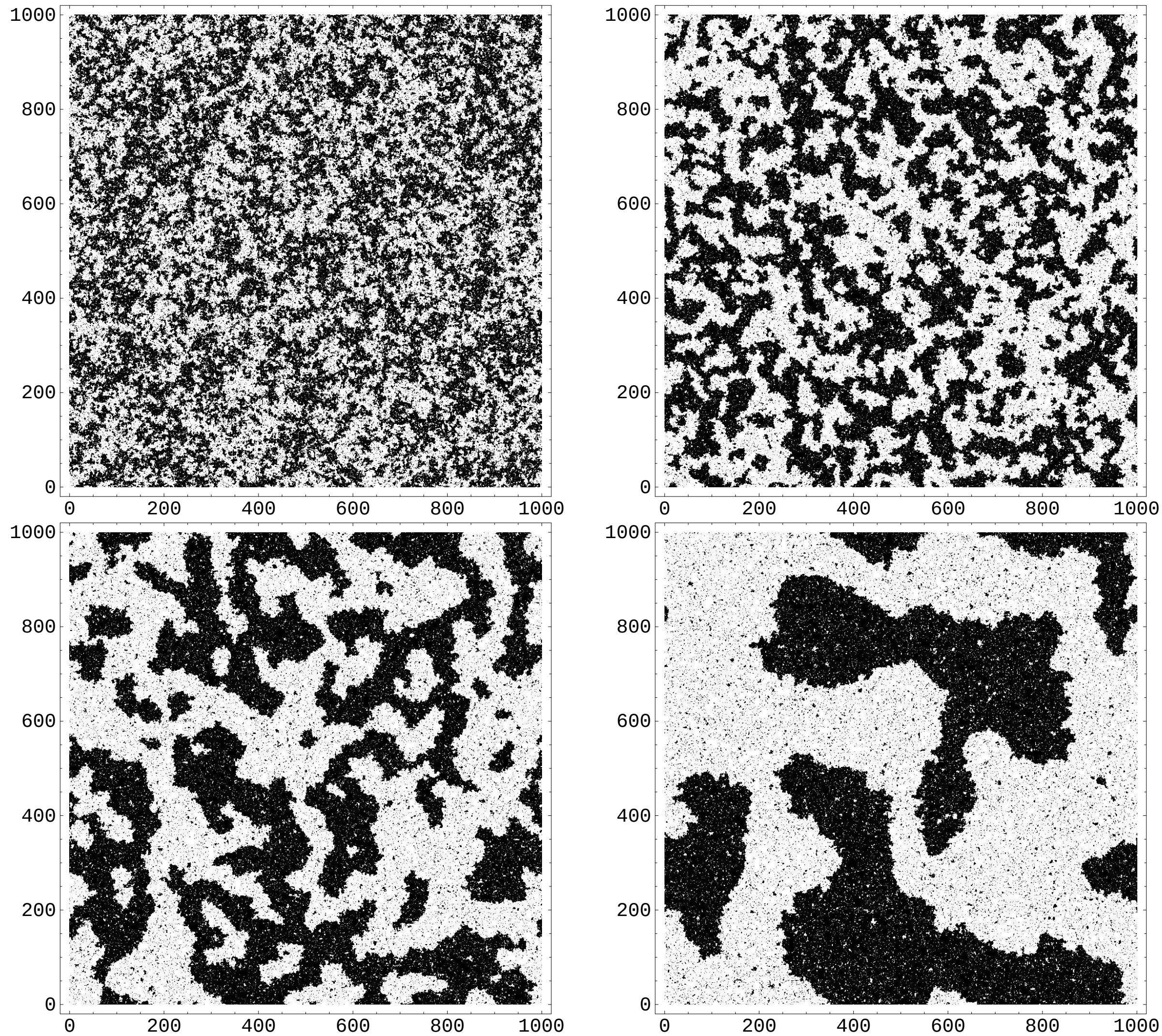

FIG. 36: Patterns of spins in the Ising model slighly above $T_c \simeq 2.269\ldots$ (top left, $T = 2.4$) and below T_c at $T = 2.1$ at different times $t = 3$ (top right), $t = 13$ (lower left) and $t = 130$ (lower right).

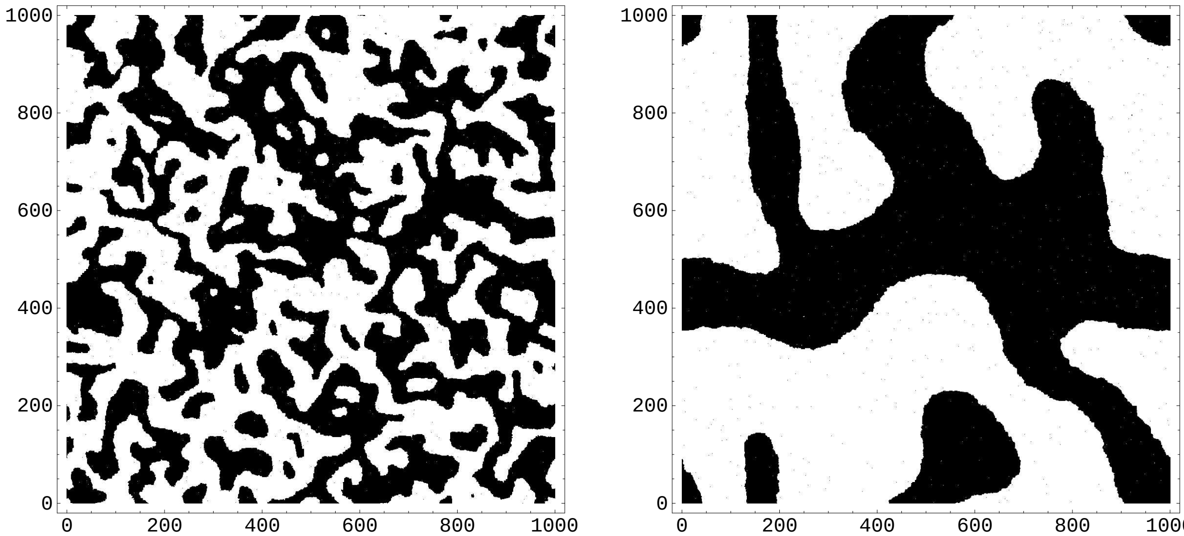

FIG. 37: Same, but at colder temperature $T = 1.1$.