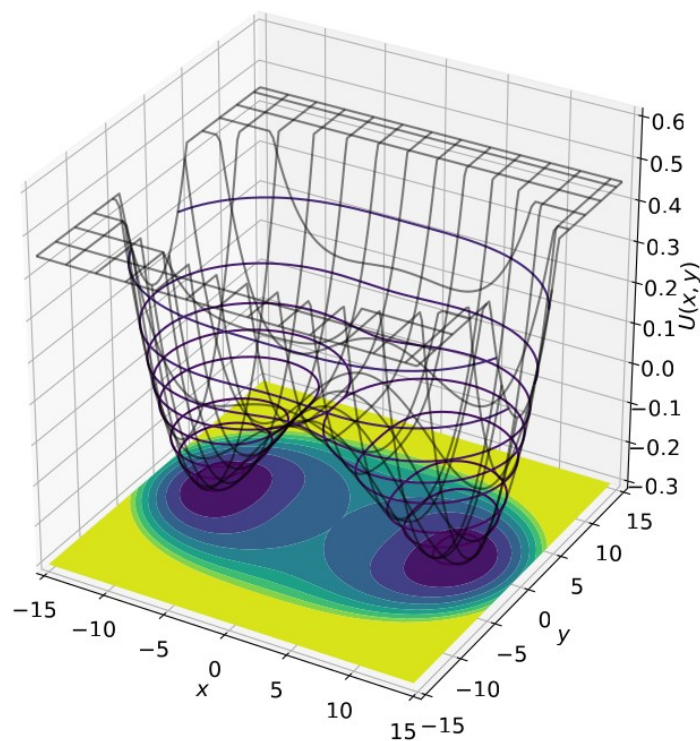


ІІТМО

М.И. Петров, И.В. Рожанский, И.Д. Тофтул

COMPUTER MODELING IN PHYSICS. APPLICATIONS



**Санкт-Петербург
2022**

МИНИСТЕРСТВО НАУКИ И ВЫСШЕГО ОБРАЗОВАНИЯ РОССИЙСКОЙ
ФЕДЕРАЦИИ

УНИВЕРСИТЕТ ИТМО

М.И. Петров, И.В. Рожанский, И.Д. Тофтул
COMPUTER MODELING IN PHYSICS.
APPLICATIONS

УЧЕБНО-МЕТОДИЧЕСКОЕ ПОСОБИЕ

РЕКОМЕНДОВАНО К ИСПОЛЬЗОВАНИЮ В УНИВЕРСИТЕТЕ ИТМО
по направлению подготовки 16.03.01. Техническая физика
в качестве Учебно-методического пособия для реализации основных
профессиональных образовательных программ высшего образования
бакалавриата

ИТМО

Санкт-Петербург
2022

Петров М.И., Рожанский И.В., Тофтул И.Д., Computer modeling in physics. Applications — СПб: Университет ИТМО, 2022. — 34 с.

Рецензент(ы):

Лосев Александр Сергеевич, к.ф.-м.н., доцент кафедры общей физики-1, СПбГУ;

This course is aimed to achieve several goals:

1. Recall basic coding skill and main methods of solving differential equations and more.
2. Learn about the most popular and models of epidimiology, numerical approach to Schrödinger and Maxwell equations, optical trapping and stochastic force imulation, and the theory of percolation.
3. Present information in informative, clear and beautiful way. Consider eash assignment as a small research.
4. Learn how to set meaningful constants in each model.

The logo of ITMO University, consisting of the letters 'ITMO' in a bold, black, sans-serif font. The letter 'I' has a small dot above it.

Университет ИТМО – ведущий вуз России в области информационных и фотонных технологий, один из немногих российских вузов, получивших в 2009 году статус национального исследовательского университета. С 2013 года Университет ИТМО – участник программы повышения конкурентоспособности российских университетов среди ведущих мировых научно-образовательных центров, известной как проект «5 в 100». Цель Университета ИТМО – становление исследовательского университета мирового уровня, предпринимательского по типу, ориентированного на интернационализацию всех направлений деятельности.

© Университет ИТМО, 2022

© Петров М.И., Рожанский И.В., Тофтул И.Д., 2022

Contents

| | | |
|----------|--|-----------|
| 1 | Zombie apocalypse! | 5 |
| 1.1 | Standard SIR model | 5 |
| 1.2 | Zombies attack! | 7 |
| 1.2.1 | Problem statement | 7 |
| 1.3 | Report requirements | 8 |
| 2 | Optical tweezers and thermal noise | 9 |
| 2.1 | Optical tweezers, or the Nobel Prize in physics (2018) | 9 |
| 2.2 | How to treat a stochastic force | 12 |
| 2.2.1 | So what is the problem? | 12 |
| 2.2.2 | What do we know about stochastic force | 12 |
| 2.2.3 | How to work with stochastic force | 14 |
| 2.3 | Two optical traps located next to each other | 15 |
| 2.4 | References | 16 |
| 3 | Quantum well | 18 |
| 3.1 | Particle in a box | 19 |
| 3.2 | Step 1: Numerical solution of Schrödinger equation | 19 |
| 3.2.1 | Discretization | 19 |
| 3.2.2 | Benchmark | 21 |
| 3.3 | Step 2: Individual assignments | 21 |
| 3.3.1 | Particle in a one-dimensional lattice | 21 |
| 3.3.2 | Hydrogen atom | 22 |
| 4 | Theory of percolation | 23 |
| 4.1 | Background | 23 |
| 4.2 | 3D percolation model for conductivity | 24 |
| 4.3 | Problem statement | 26 |
| 4.4 | References | 26 |
| 5 | Fermi energy level | 27 |
| 5.1 | Some theory | 27 |
| 5.2 | Things to do | 28 |

| | | |
|----------|--|-----------|
| 6 | Planar waveguide | 29 |
| 6.1 | Planar step-index waveguide | 29 |
| 6.2 | Simple ray approximation | 30 |
| 6.3 | Rigorous approach. Photon trapped in an inverse well formed by a non-uniform refractive index | 31 |
| 6.4 | Assignments | 33 |
| 6.5 | References | 34 |

Lab 1. Zombie apocalypse!

by Ivan Toftul

Abstract

This introductory is aimed to achieve several goals:

1. Recall basic coding skills and the main methods for solving differential equations.
2. Learn about “flow” models based on an empirically developed system of differential equations. Such systems are useful if one needs to describe population dynamics, epidemic spread, biological reactions, or even money flows in finance. Here, we consider a basic model from epidemiology as theoretical foundation.
3. Present information in an informative, clear and beautiful way.
4. Learn how to set meaningful constants in a model.

The final task is to consider zombie apocalypse using the developed approach. Consider this as a small research.

1.1 Standard SIR model

Suppose we are to describe the dynamics of a disease spreading within a large group of people. Instead of watching individuals, we can meet this task using a relatively simple system of ordinary differential equations (ODE). Let us start with one of the conventional models in epidemiology¹, the SIR model (**S**usceptible-**I**nfected-**R**ecovered). It implies classifying all the people considered into three categories:

1. Susceptible people. People who don't have any immunity to the disease.

¹Some ideas are taken from the online course “Differential equations in action” on Udacity platform.

2. Infected people. Those who are affected by the disease and may infect other people.
3. Recovered people. People who have already recovered and are immune.

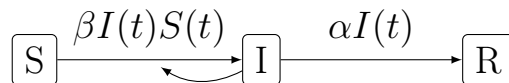


Figure 1.1: Basic SIR model.

Fig. 1.1 is a graph of a basic SIR model. Mathematically, we can write a system of *non-linear* ODEs, which is equivalent to the graph above:

$$\begin{cases} \dot{S}(t) = -\beta I(t)S(t) \\ \dot{I}(t) = \beta I(t)S(t) - \alpha I(t) \\ \dot{R}(t) = \alpha I(t) \end{cases} \quad (1.1)$$

Interestingly, the second equation can be rewritten as $\dot{I} = (\beta IS - \alpha) I$: thus, if the expression in the parentheses is negative, there is no epidemic! This effect is called **herb immunity**. Here, we have used the following assumptions:

1. No spacial distribution. We have no information about the geographical location of the infected people.
2. Variables for the number of people are non-integer.
3. Infinite immunity. The recovered never get infected again.

Some notes about the constants:

- Recovery rate $[\alpha] = [1/\text{day}]$. Note that α^{-1} is the average recovery time.
- Transmission coefficient $[\beta] = [\frac{1}{\text{day} \cdot \text{person}}]$. To identify it, we have to know the average number of people each person sees per day, the total number of susceptible and infected people, and the probability of becoming infected.

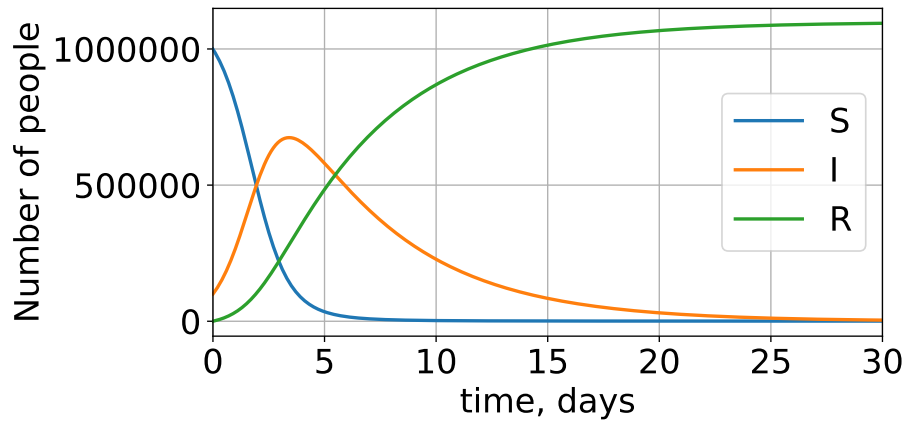


Figure 1.2: Typical behavior of a SIR model. The number of the infected has a clear peak.

1.2 Zombies attack!

1.2.1 Problem statement

For your lab report, consider a zombie apocalypse model, which has the same principles as in a SIR model. The starting point of the model is shown schematically in Fig. 1.3.

Here, we assume that there are four types of “people”:

1. **Susceptible.** Just ordinary people who may become infected. They may as well die of old age.
2. **Infected.** Those people have been bitten by zombies, and after a while, they become zombies themselves. However, they can still fight against zombies, because they are sane.
3. **Zombies.** Not particularly smart creatures. They just want more fresh meat.
4. **Dead.** Once you are dead, there is no way you may come back.²

Let us suppose that there is a group of scientists who were working hard to create an antidote. After $T_{\text{antidote}} = 100$ days, they succeeded! We can take this into account as B coefficient

$$B(t) = \begin{cases} 0, & t < T_{\text{antidote}} \\ \neq 0, & t \geq T_{\text{antidote}} \end{cases} \quad (1.2)$$

²Well, actually it is up to you what kind of zombies you want.

Here, we have developed a basic minimal model. For inspiration, you can read this paper³, which considers various models and provides analysis.

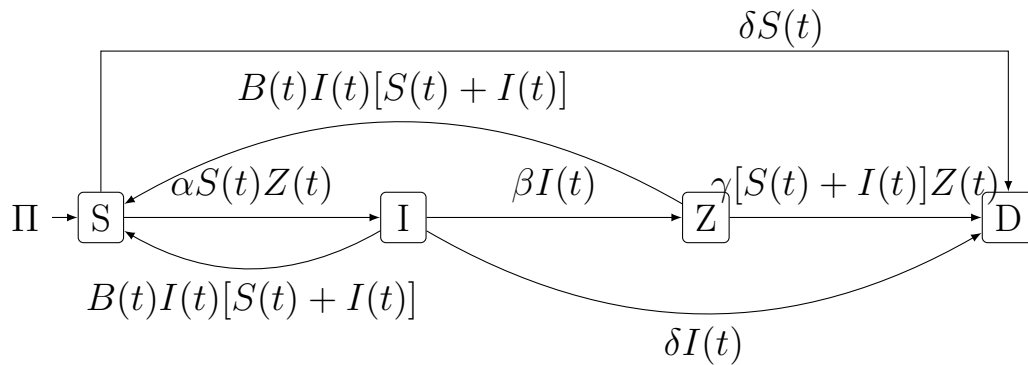


Figure 1.3: The starting point of a zombie apocalypse model.

1.3 Report requirements

1. Consider this as a small research. It is better to have fewer plots but more analysis. Make it 2-3 pages long.
2. It is up to you to choose the proper constants, however they should make sense.
3. You can change the model if you really want to.
4. You have to understand what is going on both in your text and in the code.
5. You have to be able to change your code if I add or remove a link in the diagram.
6. Make the report in \LaTeX . Believe me, it is a very useful tool.
7. You are free to use any numerical methods. However, it is preferable to use `Python`, since in the second lab, we will definitely use it for interactivity.

³Munz, Philip, et al. "When zombies attack!: mathematical modelling of an outbreak of zombie infection." *Infectious disease modelling research progress* 4 (2009): 133-150.

Lab 2. Optical tweezers and thermal noise

by Ivan Toftul

Abstract

The main goal of this work is to learn how to deal with a **stochastic force**. We will see why the straightforward approach fails and how the fluctuation-dissipation theorem helps. As an example, we will consider a dynamic simulation of a trapped particle in optical tweezers with **thermal noise**.

2.1 Optical tweezers, or the Nobel Prize in physics (2018)

In this lab work, we are going to consider nanoparticle trapping with optical tweezers as an example of a real life application. Optical tweezers have become an essential and a versatile tool in physics, biology and chemistry. Optical tweezers allow people to gently manipulate *subwavelength* objects in all three dimensions. Apart from physical manipulation, moving objects using light is extremely caring and non-destructive for the object itself.

To learn how optical tweezers work, we start with the optical force. A subwavelength particle in an external field \mathbf{E} has the induced dipole moment \mathbf{p} only. From the energy point of view, we can write the dipole optical force as¹

$$\mathbf{F}_{\text{grad}} = -\nabla U = \nabla (\mathbf{p} \cdot \mathbf{E}). \quad (2.1)$$

Usually, small particles have no internal dipole moment, and thus, \mathbf{p} is a dipole moment *induced* by the external field. Introducing polarizability

¹This is the gradient optical force, which does not take in account the light pressure and is defined only in the real (not complex) domain.

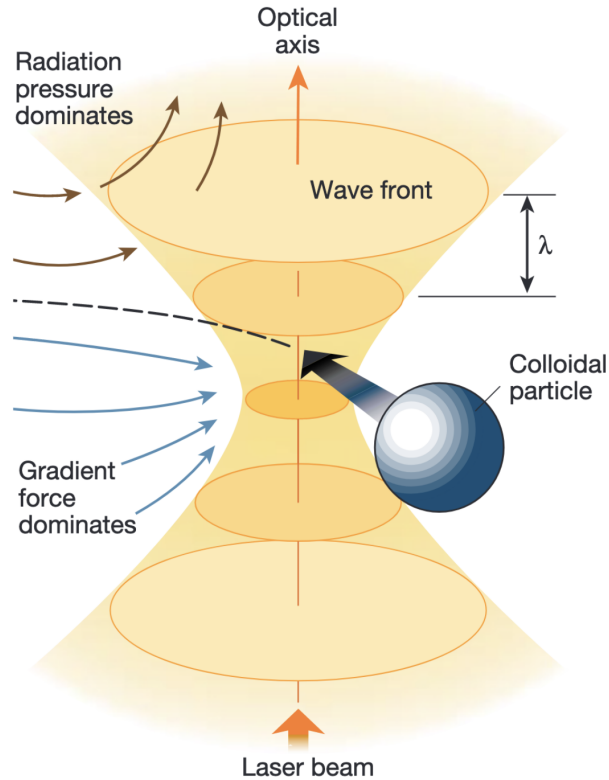


Figure 2.1: Optical tweezing by tightly focused light. The particle is drawn towards the higher-intensity region since $\mathbf{F}_{\text{grad}} = \alpha \nabla (E^2)$. Near the beam center, this force can be approximated by a linear function as $F_{\text{grad},\rho} = -\kappa\rho$. Image is taken from [David G. Grier *Nature* **424**, 810–816 (2003)].

α as a linear response function $\mathbf{p} \stackrel{\text{def}}{=} \alpha \mathbf{E}$, we can rewrite the force as

$$\mathbf{F}_{\text{grad}} = \alpha \nabla (E^2). \quad (2.2)$$

This expression is easier to analyze. First, all the information about the particle is stored in its polarizability α . Second, the dipole particle is attracted by the higher-intensity regions, or to the focal spot of the optical tweezers (Fig. 2.1). A focused beam can be described as a *Gaussian beam*², whose field is $E \propto e^{-\rho^2/w^2}$, where w is the beam waist and ρ is the distance from the center of the beam. We introduce these parameters into (2.2) and expand the latter into Taylor series up to the first order to obtain the approximate radial component of the optical gradient force

$$F_{\text{grad},\rho} = -\kappa\rho. \quad (2.3)$$

Here, κ is the stiffness of the optical trap³. This is a very simple linear law, but still, it is powerful enough to describe the effect.

²See, for example, *Gaussian Beams* by Maria Deinerowitz

³Usually, exactly this parameter is measured experimentally.

It is the the dynamic of the particle that is of interest to us. Thermal noise appears to be a serious experimental issue, which has to be taken into account. Hence, the final equation of motion reads as

$$m\ddot{\mathbf{r}} = -\zeta\dot{\mathbf{r}} + \mathbf{F} + \mathbf{F}_{\text{grad}}, \quad (2.4)$$

where ζ is viscosity constant and \mathbf{F} is the stochastic force, which originates from numerous collisions with smaller particles in the host fluid/air (Brownian motion).

Here, we emphasize that once there is a viscosity force (which leads to dissipation), there is a stochastic force **always** present. This two terms are fundamentally interrelated by the *fluctuation-dissipation theorem*. This can be explained by the fact that both friction and Brownian motion are caused by the numerous collisions with atoms in the host fluid (a gas is also a fluid).

In this work, we are going to consider a tricky example of two optical tweezers located nearby. Due to the thermal noise in the system, a trapped particle could be unstable and “tunnel” from one trap to another. An example of such simulation is shown in Fig. 2.2.

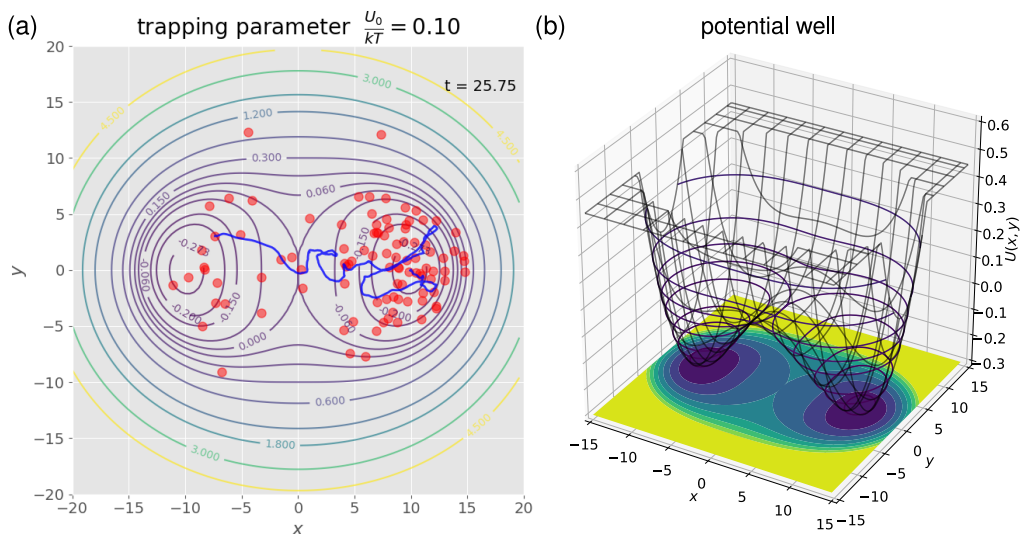


Figure 2.2: Simulation of optical trapping with thermal noise. (a) Each red dot represents a different implementation of particle trapping (there is no interaction between the particles). At $t = 0$, all particles are in the right-hand trap, and then, due to thermal fluctuations, some of them jump to the second trap (i.e. the left-hand trap). (b) Toy-model potential for two optical tweezers located nearby.

2.2 How to treat a stochastic force

2.2.1 So what is the problem?

We start with Langevin equation⁴

$$m\ddot{\mathbf{r}} = -\zeta\dot{\mathbf{r}} + \mathbf{F} \quad (2.5)$$

which can be rewritten in terms of only first order differential equations (DE) as

$$\begin{cases} \dot{\mathbf{r}} = \mathbf{v}, \\ \dot{\mathbf{v}} = -\frac{\zeta}{m}\mathbf{v} + \frac{1}{m}\mathbf{F}. \end{cases} \quad (2.6)$$

Now we use a numeric approach to this system of DEs. Let us solve it with a discrete time step $\Delta t = t_{i+1} - t_i$. The straightforward approach

$\int_{t_i}^{t_{i+1}} (2.6)dt$ using Euler method gives us

$$\begin{cases} \mathbf{r}_{i+1} = \mathbf{r}_i + \Delta t\mathbf{v}_i, \\ \mathbf{v}_{i+1} = \mathbf{v}_i - \Delta t\frac{\zeta}{m}\mathbf{v}_i + \frac{1}{m}\int_{t_i}^{t_{i+1}} \mathbf{F}(t)dt \neq \left(1 - \frac{\zeta}{m}\Delta t\right)\mathbf{v}_i + \frac{1}{m}\mathbf{F}_i\Delta t \end{cases} \quad (2.7)$$

where $\mathbf{r}_i \equiv \mathbf{r}(t_i)$. The latter equation cannot be approximated by the Mean-Value theorem (see [Ko, Stanley. "Mathematical analysis." (2006)]) because the stochastic force function $\mathbf{F}(t)$ is a non-smooth function and cannot be expanded in Taylor series. This means that

$$\int_{t_i}^{t_{i+1}} \mathbf{F}(t)dt \neq \mathbf{F}_i\Delta t. \quad (2.8)$$

Equation (2.8) contains the main problem which we have to address. The trick is to treat this integral as a whole. In the following subsection we will learn about its properties.

2.2.2 What do we know about stochastic force

All we know about a stochastic force \mathbf{F} is that in average it is zero, and at each moment in time, it is independent from the past (white noise). Mathematically, this can be written as

$$\langle \mathbf{F}(t) \rangle_t = 0, \quad (2.9)$$

$$\langle F_\alpha(t)F_\beta(t+\tau) \rangle_t = 2D\delta_{\alpha\beta}\delta(\tau), \quad (2.10)$$

⁴Some ideas are taken from the edx.org online course "Stochastic Processes: Data Analysis and Computer Simulation" by Kyoto University.

where $\langle f(t) \rangle_t \stackrel{\text{def}}{=} \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-T/2}^{T/2} dt f(t)$ and $\alpha, \beta = x, y, z$. Constant D is proportional to the **d**iffusion constant and “2” is chosen for the sake of convenience. Equation (2.10) can be written in terms of *auto-correlation function* as

$$\varphi_F(\tau) = \langle \mathbf{F}(t) \cdot \mathbf{F}(t + \tau) \rangle_t = 6D\delta(\tau). \quad (2.11)$$

All things considered, we can write

$$D = D(\zeta, T). \quad (2.12)$$

To elicit this dependency, some work has to be done. The key to the solution of this problem is thermodynamics.

First, we find the spectral density $S_F(\omega)$ of the stochastic force $\mathbf{F}(t)$, using the Wiener-Khintchine theorem⁵

$$S_F(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \varphi_F(t) = 6D. \quad (2.13)$$

Then, we find the auto-correlation function of speed $\varphi_v(t)$, because it is related to the average kinetic energy $U_{\text{kin}} \propto \varphi_v(t = 0)$. On the other hand, we do not know the exact time dependence $\mathbf{v}(t)$ yet. However, we can find $\mathbf{v}(\omega)$ instead, using Fourier transform:

$$m\dot{\mathbf{v}} = -\zeta\mathbf{v} + \mathbf{F} \quad \xrightarrow{\mathcal{F}\{\dots\}} \quad \mathbf{v}(\omega) = \frac{\mathbf{F}(\omega)}{\zeta - i\omega m}. \quad (2.14)$$

⁵For a signal function, $y(t)$ the Wiener-Khintchine theorem reads as:

$$\varphi_y(\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} S_y(\omega).$$

It states that the auto-correlation and spectral density functions are connected through Fourier transform.

Spectral density of the velocity is given by⁶

$$S_v(\omega) = \lim_{T \rightarrow \infty} \frac{1}{T} |\mathbf{v}(\omega)|^2 = \frac{1}{\zeta^2 + m^2 \omega^2} \lim_{T \rightarrow \infty} \frac{1}{T} |\mathbf{F}(\omega)|^2 = \frac{6D}{\zeta^2 + m^2 \omega^2}. \quad (2.15)$$

Applying Wiener-Khintchine theorem, we finally get

$$\varphi_v(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} S_v(\omega) = \frac{3D}{\zeta m} \exp\left(-\frac{\zeta}{m}|t|\right). \quad (2.16)$$

Finally, we note that $\varphi_v(t=0) = \langle \mathbf{v}^2 \rangle$. In other words,

$$\langle U_{\text{kin}} \rangle = \frac{m \langle \mathbf{v}^2 \rangle}{2} = \left/ \text{from thermodynamics} \right/ = 3 \cdot \frac{kT}{2}, \quad (2.17)$$

and thus, the solution to Eq. (2.12) is:

$$D = kT\zeta. \quad (2.18)$$

2.2.3 How to work with stochastic force

The trick is to introduce a new variable

$$\int_{t_i}^{t_{i+1}} dt \mathbf{F}(t) \equiv \Delta \mathbf{W}_i(t). \quad (2.19)$$

Let us look at its properties:

$$\begin{aligned} \langle \Delta \mathbf{W}_i \rangle &= 0 \quad (2.20) \\ \langle \Delta \mathbf{W}_i \cdot \Delta \mathbf{W}_j \rangle &= \delta_{ij} \int_{t_i}^{t_{i+1}} dt_1 \int_{t_i}^{t_{i+1}} dt_2 \langle \mathbf{F}(t_1) \cdot \mathbf{F}(t_2) \rangle = \delta_{ij} \cdot 6kT\zeta \end{aligned}$$

⁶For a signal function, $y(t)$ we have (proof of the Wiener-Khintchine theorem)

$$\begin{aligned} \varphi_y(\tau) &\stackrel{\text{def}}{=} \langle y(t)y(t+\tau) \rangle_t = \lim_{T \rightarrow \infty} \int_{-\infty}^{\infty} dt \left[y(t) \left(\int \frac{d\omega}{2\pi} e^{-i\omega(t+\tau)} y(\omega) \right) \right] = \\ &= \lim_{T \rightarrow \infty} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left[e^{-i\omega\tau} y(\omega) \int_{-\infty}^{\infty} dt (e^{-i\omega t} y(t)) \right] = \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} y(\omega) y^*(\omega) = \\ &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} \underbrace{\left[\lim_{T \rightarrow \infty} \frac{1}{T} |y(\omega)|^2 \right]}_{\equiv S_y(\omega)} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} S_y(\omega). \end{aligned}$$

Since $\langle \Delta \mathbf{W}_i \rangle = 0$, Eq. (2.21) is just the dispersion σ^2 of $\Delta W_i(t)$. This gives the answer to question of this section: ΔW is a normally⁷ distributed random value with the dispersion **that depends on the time step Δt** :

$$\sigma = \sqrt{2kT\zeta\Delta t}. \quad (2.22)$$

Comments

References provide a different but *equivalent* approach can be found [3]. The equation of motion can be integrated as

$$\int_{t_i}^{t_{i+1}} dt \mathbf{F}(t) \equiv \mathbf{R}(t) \Delta t, \quad (2.23)$$

where $\mathbf{R}(t)$ is a normally distributed random function with the dispersion $\sigma = \langle \mathbf{R} \cdot \mathbf{R} \rangle$, which has a different dependence on the time discretization step:

$$\langle \mathbf{R} \cdot \mathbf{R} \rangle = \sqrt{\frac{2kT\zeta}{\Delta t}}. \quad (2.24)$$

Please note that this approach gives exactly the same result as the one described above. You can find the exact derivation in [4].

2.3 Two optical traps located next to each other

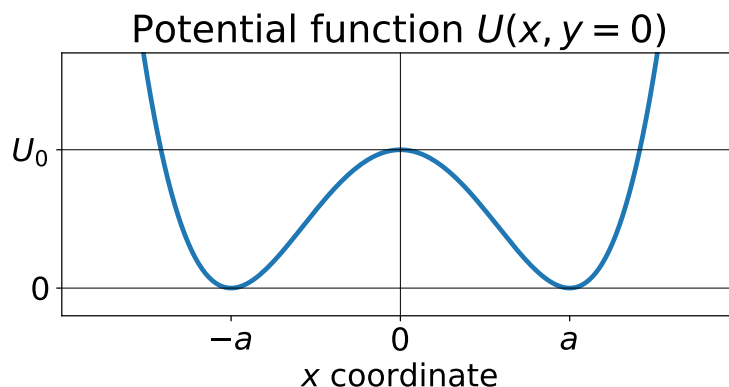


Figure 2.3: Toy-model potential with clearly indicated parameters: the depth of the potential well U_0 and the distance between the minima a .

⁷Usually, all processes in nature are normally distributed.

Now we have everything we need to formulate the problem for the report. You have to consider *two* optical traps next to each other. To do this, follow the steps:

1. Consider only the 2D motion for the sake of simplicity.
2. Design a toy-model potential for two traps $U(x, y)$ (see the example in Fig. 2.2 (b)). Remember that since the force is linear near the trap's center $F_{\text{grad},\rho} = -\kappa\rho$, the potential should be quadratic near each minimum, similar to a single trap $U_{\text{single trap}} = \frac{\kappa\rho^2}{2}$. A good way to start is a fourth-order polynomial. Write the potential in a form which is easy to analyze, and make these parameters explicitly visible:
 - (a) U_0 — depth of the potential well.
 - (b) a — distance between the two minima.

These parameters are shown in Fig. 2.3.

3. Add the gradient force into Langevin equation (2.5) in the form $\mathbf{F} = -\nabla U(x, y)$.
4. Treat the stochastic force properly!
5. Simulate the motion of a particle trapped by two optical tweezers. At this step, do not use the real constants, do it in *arbitrary units*. By tuning the temperature, find different regimes of particle motion:
 - (a) The particle is trapped only in one potential well.
 - (b) The particle jumps from one trap to another, as the temperature is too high to obtain any stable trapping.
 - (c) Critical behavior.

Change only one dimensionless parameter U_0/kT .

6. (*extra*) Figure out the real parameters of the problem.

2.4 References

1. Jacobs, Kurt. Stochastic processes for physicists: understanding noisy systems. Cambridge University Press, 2010.
2. “Stochastic Processes: Data Analysis and Computer Simulation” by Kyoto University.

3. Karpov, S. V., et al. "General principles of the crystallization of nanostructured disperse systems." Colloid journal 71.3 (2009): 313-328.
4. Heermann, Dieter W. "Computer-simulation methods." Computer Simulation Methods in Theoretical Physics. Springer, Berlin, Heidelberg, 1990. 8-12.

Lab 3. Quantum well

by Igor Rozhansky

Abstract

In this lab work, we will focus on the 1D stationary Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

or

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right] \psi(x) = E\psi(x).$$

We will use a standard discretization method and consider various potential functions $U(x)$ and boundary conditions.

There are two tasks for everyone:

1. (The same for everyone) Find the first few energy levels for an electron in a box.
2. Some individual assignments.



3.1 Particle in a box

We start with a problem that has an analytical solution. Consider an electron with the mass m that can travel in the x direction. This electron is confined between infinitely high potential walls (Fig. 3.1)

$$U(x) = \begin{cases} 0 & \text{if } x \in (-a/2, a/2) \\ +\infty & \text{else} \end{cases} \quad (3.1)$$

The electron follows Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right] \psi(x) = E\psi(x). \quad (3.2)$$

This toy model, usually referred to as *particle in a box*, has an analytical solution. Applying proper boundary conditions

$$\psi(-a/2) = \psi(a/2) = 0 \quad (3.3)$$

we can obtain the eigenfunctions (wave function) and eigenvalues (energy spectrum) of the electron

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n x}{a} + \frac{\pi n}{2}\right), \quad E_n = \frac{\pi^2 \hbar^2 n^2}{2ma^2}. \quad (3.4)$$

The solution is shown in Fig. 3.1.

3.2 Step 1: Numerical solution of Schrödinger equation

Here, we deal with the first assignment of this lab work. Our main goal is to solve Eq. (3.2) for any potential function $U(x)$. To do this, we have to *discretize* our problem, using the finite-difference method (**not** to be confused with the finite element method). The key step here is to discretize our space and rewrite the derivative using finite steps.

3.2.1 Discretization

The finite-difference method is based on the approximation of the derivatives for a discrete set of values $\{x_n\}_N$ (instead of a continuous x) with the step Δx (see Fig. 3.2).

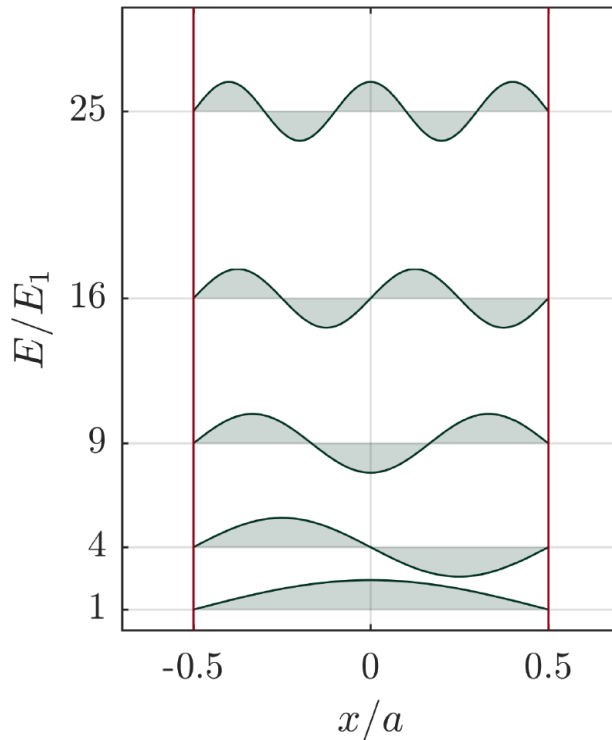


Figure 3.1: Potential function with infinitely high walls. This problem has an analytical solution: the energy levels of the electron are discrete and equal to $E_n = \pi^2 \hbar^2 n^2 / (2ma^2)$.

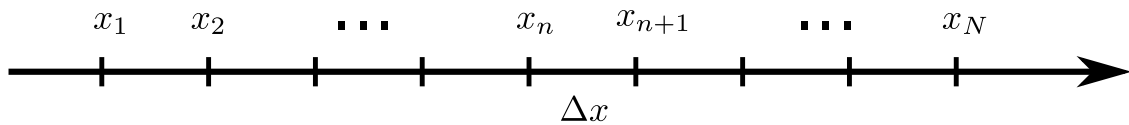


Figure 3.2: Discretization of the x axis. Instead of a continuous x , we have a set of $\{x_n\}_N$.

In this case, instead of continuous functions themselves, we will work only with their particular values at certain predefined positions (which are given by $\{x_n\}_N$):

$$\psi(x) \rightarrow \{\psi_n\}_N \equiv \{\psi(x_n)\}_N, \quad (3.5)$$

$$U(x) \rightarrow \{U_n\}_N \equiv \{U(x_n)\}_N. \quad (3.6)$$

We can approximate the derivatives by applying *central differencing*:

$$\frac{d\psi(x_n)}{dx} \approx \frac{\psi_{n+1} - \psi_{n-1}}{2\Delta x}, \quad (3.7)$$

$$\frac{d^2\psi(x_n)}{dx^2} \approx \frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{\Delta x^2}. \quad (3.8)$$

The latter equation is obtained by applying the first derivative twice using centered differencing, or else from Taylor expansion (e.g., see [D. Levy Numerical Differentiation](#)). Thus, we can rewrite Schrödinger equation

in this new discrete space as

$$-\frac{\hbar^2}{2m} \frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{\Delta x^2} + U_n \psi_n = E \psi_n, \quad (3.9)$$

which can be solved in a matrix form.

3.2.2 Benchmark

To verify this approach, use the analytical solution (3.4) as a benchmark.

Thus, you have to do the following:

1. Use dimensionless variables.
2. Solve the discrete Schrödinger equation (3.9) using any available matrix solver.
3. Figure out how to treat boundary conditions.
4. Compare your solution to the well-known analytical solution (3.4).
5. Double-check the normalization of the wave function. Remember, you should always have

$$\int \psi(x) dx = 1. \quad (3.10)$$

3.3 Step 2: Individual assignments

To complete this lab work, you are also to solve **one** of the following problems.

3.3.1 Particle in a one-dimensional lattice

Consider a different number of potential wells, as shown in Fig. 3.3, and analyze the dispersion curves $E(k)$. You are to:

1. Consider a finite number of wells ($M \gg 1$).
2. Compare your results to the analytical solution for the infinite number of potential wells (refer to Kronig–Penney model¹).

¹See the references:

- [Kronig, Penney \(1931\)](#).
- [Short tutorial on Kronig-Penney model](#).
- [Pavel Exner, PRL \(1995\)](#).

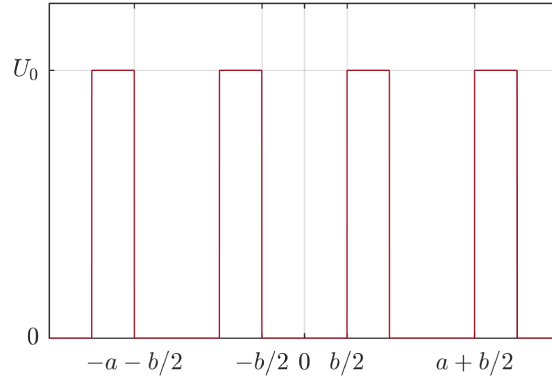


Figure 3.3: Periodic potential. Here, a is the period, b is the width of the well, U_0 is the depth.

3.3.2 Hydrogen atom

Solve Schrödinger equation for a hydrogen atom in spherical coordinates

$$\left(-\frac{\hbar^2}{2\mu} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \right) \psi(r, \theta, \phi) = E\psi(r, \theta, \phi). \quad (3.11)$$

Expanding the Laplacian in spherical coordinates, we have

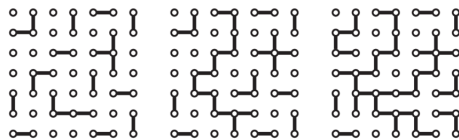
$$\begin{aligned} & -\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] \\ & - \frac{e^2}{4\pi\epsilon_0 r} \psi = E\psi. \end{aligned} \quad (3.12)$$

Compare the result to the well-known analytical solution (see the solution for the hydrogen atom in quantum mechanics textbooks, e.g. in [Flügge, Siegfried. *Practical quantum mechanics*. Springer Science & Business Media, 2012]).

Lab 4. Theory of percolation

by Igor Rozhansky

Abstract



4.1 Background

Percolation theory is a relatively young branch of science. Its basic ideas were formulated in 1957 in a paper by two British scientists, S. R. Broadbent and J. M. Hammersley. During the mid-1950's, Broadbent was working at the British Coal Utilization Research Association, designing gas masks to use in coal mines. He encountered across an interesting problem and presented it to the mathematician Hammersley.

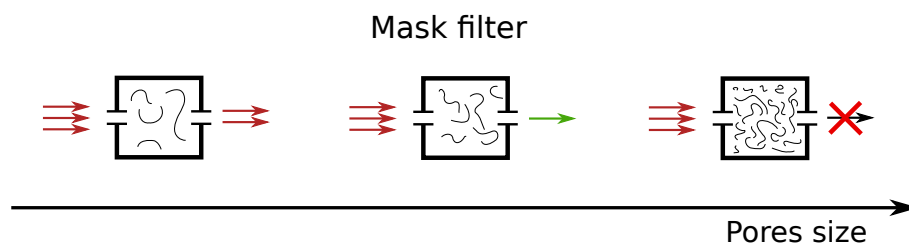


Figure 4.1: Initial problem of the percolation theory. There is an optimal size of the mask pores.

The problem was as follows. The principal element of a mask is filled with carbon granules through which the gas flows. Carbon contains pores that are connected in an intricate manner, forming a sophisticated maze. A gas can enter the pores by being adsorbed on their inner surface. The scientists discovered a tricky interplay of parameters where they had

to find the balance: on the one hand, if the pores are wide and well-connected, the gas penetrates deep into the carbon filter, and the mask does not protect enough; on the other hand, for small and narrow pores, the gas cannot get beyond the outer surface of the carbon, and a worker cannot breath (Fig. 4.1). The motion of a gas through the maze is a new type of process, different from diffusion.

Broadbent and Hammersley called the phenomenon *percolation*, and the theory describing the processes of this type is called the *percolation theory* [1]. The phenomena best described by percolation theory are *critical phenomena*. They are characterized by a critical point when the properties of the system abruptly change.

4.2 3D percolation model for conductivity

In this work, we will focus on a particular example of the percolation theory: Miller-Abrahams resistance grid [2].

Let us consider a 3D cube with edge length L . Inside that cube, there are N *randomly* positioned nodes. The conductivity σ_{ij} between the nodes i and j is defined by exponential decay:

$$\sigma_{ij} = \sigma_0 e^{-\gamma r_{ij}}, \quad r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|. \quad (4.1)$$

Here, σ_0 is the conductivity and γ is the inverse interaction distance. Self-conductivity has no physical meaning in this problem, and hence, it is equal to zero $\sigma_{ii} \equiv 0$.

On the two sides of the cube, there are conductive contacts with electric potential difference U (Fig. 4.2). **The objective** of this work is to calculate the resistance between these two sides of the cube as a function of the average distance between the conducting nodes. Naively, we could predict that the total conductivity would be

$$\sigma_{\text{total}}(\langle d \rangle) = \tilde{\sigma}_0 e^{-\gamma \langle d \rangle}, \quad (4.2)$$

where $\langle d \rangle$ is the average distance between the nodes. However, we will see that is not true.

To simulate the conductivity between the two contact surfaces given that all the nodes are randomly located, we introduce two thin volumes as shown on Fig. 4.2, and set a particular electric potential: $\varphi_i = 0$ or $\varphi_i = U$ for each node. It means that all the nodes can be classified into three groups:

1. $\varphi_j = 0$, $j \in \{j\}_{\text{in}}$ — nodes on the left side of the cube, or **in-nodes**.

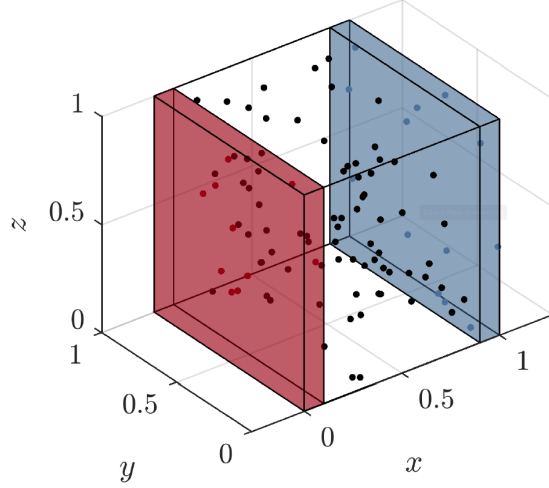


Figure 4.2: Model of Miller-Abrahams resistance grid. Two conductive contacts of the cube are represented as red and blue volumes. Inside each contact all nodes have the same electric potential. Conductivity between any two nodes follows the exponential law (4.1).

2. $\varphi_j = ?$, $j \in \{j\}_{\text{middle}}$ — nodes within the volume of the cube, or **middle-nodes** (their potential is to be calculated!).
3. $\varphi_j = U$, $j \in \{j\}_{\text{out}}$ — nodes on the right side of the cube, or **out-nodes**.

To calculate the potentials at the nodes within the cube, we use Kirchhoff's circuit laws. Namely, for the i -th node, the sum of the incoming currents is equal to the sum of the outgoing currents

$$i = 1, \dots, N : \quad \sum_{j=1}^N (\varphi_i - \varphi_j) \sigma_{ij} = 0. \quad (4.3)$$

By choosing proper indexing, Eq. (4.3) can be solved in matrix form.

The main task here is to calculate the total conductivity of the system σ_{total} , which is defined by

$$\sigma_{\text{total}} = \frac{I_{\text{total}}}{U}, \quad (4.4)$$

where I_{total} is the total current

$$I_{\text{total}} = \sum_{j \in \{j\}_{\text{in}}} \left[\sum_{i \in \{i\}_{\text{middle}}} \varphi_i \sigma_{ij} + \sum_{i \in \{i\}_{\text{out}}} U \sigma_{ij} \right] \quad (4.5)$$

The total current is equal to the sum of currents flowing from all the nodes in the left-hand contact zone (all the in-nodes).

4.3 Problem statement

To sum up, your assignment for this lab work is as follows:

1. Solve Eq. (4.3) for the system described. Plot the total conductivity as a function of the average distance $\sigma_{\text{total}} = \sigma_{\text{total}}(\langle d \rangle)$.
2. Show that the naive solution (4.2) does not work.
3. Fit your results to

$$\sigma_{\text{total}}(\langle d \rangle) = \tilde{\sigma}_0 e^{-\alpha \gamma \langle d \rangle}. \quad (4.6)$$

Here, we have introduced a new parameter α . Find all the fitting parameters.

4.4 References

1. Efros A. L. Physics and geometry of disorder. Percolation Theory. 1982.
2. Miller, Allen, and Elihu Abrahams. "Impurity conduction at low concentrations." Physical Review 120.3 (1960): 745.

Lab 5. Fermi energy level

by Igor Rozhansky

5.1 Some theory

The properties of semiconductors can be changed by doping a material with a small amount of impurity atoms. For example, a semiconductor can be doped in such a way that the donor energy level is as close as possible to the bottom of the conduction band, while the acceptor energy level is close to the upper edge of the valence band (Fig. 5.1).

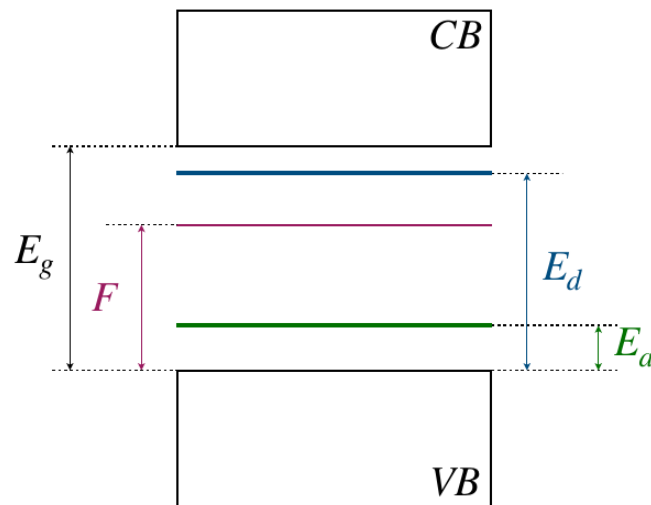


Figure 5.1: A simplified scheme of the band structure of a semiconductor doped with two types of impurities: donors and acceptors.

Let us assume that a semiconductor is doped with identical donors in N_d concentration and with acceptors (also identical) in N_a concentration. There are positive particles: positive charge carriers, i.e. holes, with the p concentration, and positively charged donors with p_t concentration.

In the case of simple donors, we have

$$\begin{cases} p_t = N_d(1 - f_d) \\ f_d = \frac{1}{1 + \exp \frac{E_d - E_F}{kT}} \end{cases} \Rightarrow p_t = \frac{N_d}{1 + \exp \frac{E_F - E_d}{kT}}, \quad (5.1)$$

where f_d is the probability that the donor is occupied with an electron, E_d is the energy level of the donor atom, and E_F is the Fermi level.

The concentration of negative particles is the sum of electrons concentration in the n -th zone and the concentration of negatively charged acceptors. If n_t is the concentration of bound elementary charges, then for the case of simple acceptors,

$$n_t = N_a f_a = \frac{N_a}{1 + \exp \frac{E_a - E_F}{kT}}, \quad (5.2)$$

where f_a is the probability that the acceptor is occupied with an electron, and E_a is the energy level of the acceptor atom.

It is noteworthy that the concentrations of electrons and holes also depend on the energy of the Fermi level as

$$n = N_c \exp \left[-\frac{E_c - E_F}{kT} \right], \quad (5.3)$$

$$p = N_v \exp \left[-\frac{E_F - E_v}{kT} \right], \quad (5.4)$$

where $N_c = 2 \left(\frac{2\pi m_n^* kT}{h^2} \right)^{3/2}$, $N_v = 2 \left(\frac{2\pi m_p^* kT}{h^2} \right)^{3/2}$, m_n^* and m_p^* are the effective masses of electrons and holes, E_c and E_v are the conduction and the valence bands edges.

Finally, we write the electrical neutrality condition as

$$p + p_t - n - n_t = 0. \quad (5.5)$$

The above *nonlinear* equation (all the four terms are nonlinear functions of the Fermi energy level E_F) is the main objective of the lab work.

5.2 Things to do

In this lab work, you have to do the following:

- Find the Fermi level of the semiconductor doped with two types of impurities (donors and acceptors).
- Explore the dependence of the Fermi level position on **one** of the parameters.

Lab 6. Planar waveguide

by Ivan Toftul

Abstract

This assignment is aimed to study the fundamental principles of waveguide theory using a specific example, planar waveguides. First, we give the simplest possible model of a waveguide, using ray approximation (the width of a waveguide \gg wavelength), which already implies a *mode concept*. Afterwards, we consider a more rigorous approach based on solving Maxwell equations. This gives a precise dispersion curve $k_z(\omega)$ and field distributions of modes. Finally, we draw an analogy between quantum mechanics and waveguide theory.

6.1 Planar step-index waveguide

In this work, we consider eigenmodes (guided modes) of a planar step-index waveguide, as shown in Fig. 6.1. In the general case, a waveguide can be asymmetric, and its permittivity changes as

$$\varepsilon(x) = \begin{cases} \varepsilon_1, & x < 0 \\ \varepsilon_2, & 0 \leq x \leq a \\ \varepsilon_3, & x > a \end{cases} \quad (6.1)$$

When $\varepsilon_1 = \varepsilon_3$, the waveguide is called symmetric.

We will show that there is a direct analogy between electron dispersion in a quantum well and photon dispersion for TE modes (transverse electric modes) in a waveguide:

$$\frac{-\hbar}{2m_e} \partial_x^2 \psi(x) + U(x) \psi(x) = E \psi(x) \Leftrightarrow \partial_x^2 E_y(x) + \varepsilon(x) k_0^2 E_y(x) = k_z^2 E_y(x) \quad (6.2)$$

where \hbar is Plank constant, m_e is the mass of the electron, ψ is the wavefunction of the electron, $U(x)$ is potential energy, E is the eigen energy

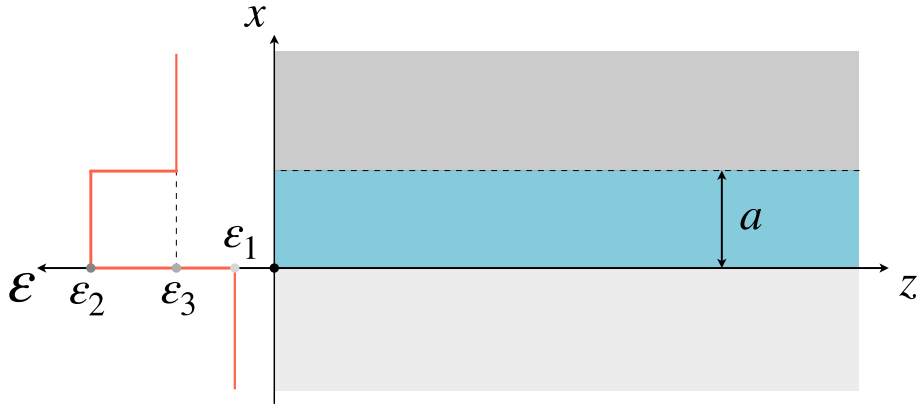


Figure 6.1: Scheme of a step-index planar waveguide. On the left, the permittivity dependence $\varepsilon(x)$ is shown. Nothing depends on the y coordinate.

of the electron; $\varepsilon(x)$ is electric permittivity, k_0 is vacuum wavenumber, k_z is guided wavevector, and E_y is the transverse component of the electric field.

6.2 Simple ray approximation

To begin with, we consider a planar waveguide in ray approximation, as shown in Fig 6.2. First, we know that if light approaches an interface with a lower refractive index medium, there is a critical reflection angle. In this case, we have a *guided mode*, which is trapped in the higher optical density region (the waveguide itself). Otherwise, the mode will not propagate far, because it will leak out of the waveguide due to transmission. Such modes are called *leaky modes*, and they are not considered further.

The condition that a guided mode exists along the entire length of the waveguide (i.e. it is an eigenmode of the system) results in certain limitations. It means that there would be no destructive interference:

$$R_{23}R_{21}e^{2ik_x a} = 1. \quad (6.3)$$

Or, in the simplest case, for $R_{23} = R_{21} = -1$, we have “quantization” of the transverse wavenumber

$$k_x = \frac{\pi m}{a} \quad (6.4)$$

and the dispersion law $k_z = k_z(\omega)$ from the triangular rule $k^2 = k_x^2 + k_z^2$ becomes

$$k_z^{\text{ray approx}}(\omega) = \sqrt{\varepsilon_2 \frac{\omega^2}{c^2} - \frac{\pi^2 m^2}{a^2}}. \quad (6.5)$$

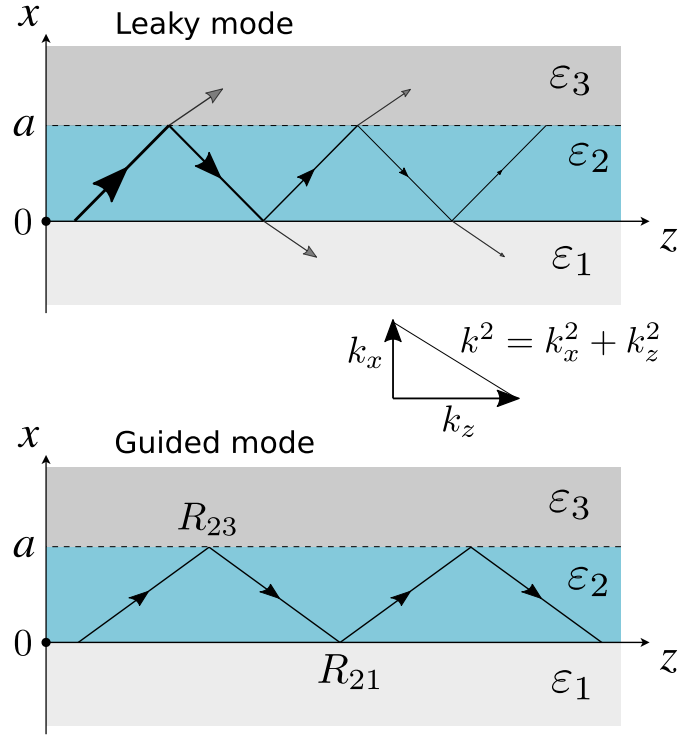


Figure 6.2: In ray approximation, we have two kinds of modes depending on the travel distance: the leaky and the guided ones. Due to the total internal reflection, a guided mode can propagate infinitely far. Here, R_{23} and R_{21} are complex Fresnel reflection coefficients.

From this formula, we see that each propagation constant k_z has its own order m . For an order that is high enough, k_z becomes purely imaginary, and such modes are not guided anymore. It means that each higher-order mode has a *cutoff frequency*!

We also emphasize that the dispersion solution in the ray approximation (6.5) is valid only for $\lambda \ll a$, where $\lambda = 2\pi/(k_0\sqrt{\epsilon_2})$ is the wavelength inside the guided region. Otherwise, we have to take into account the wave nature of the propagating modes.

6.3 Rigorous approach. Photon trapped in an inverse well formed by a non-uniform refractive index

To address the same problem rigorously, we start from the fundamental equations of electrodynamics. For a non-magnetic medium with $\mu = 1$ and no external charges or currents ($\rho = 0$ and $\mathbf{j} = 0$), Maxwell

equations in SI units are

$$\left\{ \begin{array}{l} \nabla \cdot (\varepsilon(x)\mathbf{E}) = 0 \\ \nabla \cdot \mathbf{B} = 0 \\ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \\ \nabla \times \mathbf{B} = \frac{\varepsilon(x)}{c^2} \frac{\partial \mathbf{E}}{\partial t} \end{array} \right. \quad (6.6)$$

Here, \mathbf{E} , \mathbf{B} are the electric and the magnetic fields, $c = 1/\sqrt{\varepsilon_0\mu_0}$ is the speed of light in vacuum, and $\varepsilon(x)$ is the permittivity function. Next, we simplify the equations as much as possible:

1. We consider only monochromatic fields. Since Maxwell equations are linear, we can easily use Fourier transform. In other words, we work with Fourier image of the fields. We also work in a complex domain, and thus, the real observable fields are given by

$$\boldsymbol{\mathcal{E}} = \text{Re} \{ \mathbf{E}(\mathbf{r})e^{-i\omega t} \}, \quad \boldsymbol{\mathcal{B}} = \text{Re} \{ \mathbf{B}(\mathbf{r})e^{-i\omega t} \}. \quad (6.7)$$

2. We are looking for propagating waves along the z -axis.
3. Nothing depends on the y -axis due to symmetry considerations.
4. Points 2 and 3 taken together result in the following ansatz

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}(x)e^{ik_z z}, \quad \mathbf{B}(\mathbf{r}) = \mathbf{B}(x)e^{ik_z z} \quad (6.8)$$

Summarizing all the assumptions, we can transform the Maxwell equations (6.6), using the following formal substitutions:

$$\begin{aligned} \partial_t &\rightarrow -i\omega t \\ \partial_z &\rightarrow ik_z \\ \partial_y &\rightarrow 0 \end{aligned}$$

Thus, we obtain two independent subsystems of equations

$$\begin{aligned} -\partial_z E_y &= i\omega B_x & -\partial_z B_y &= -\frac{i\omega\varepsilon(x)}{c^2} E_x \\ \partial_x E_y &= i\omega B_z & \partial_x B_y &= -\frac{i\omega\varepsilon(x)}{c^2} E_z \\ \frac{-i\omega\varepsilon(x)}{c^2} E_y &= \partial_z B_x - \partial_x B_z & i\omega B_y &= \partial_z E_x - \partial_x E_z \end{aligned} \quad (6.9)$$

These subsystems are responsible for different types of eigenmodes: transverse electric (TE) and transverse magnetic (TM), respectively. For TE and TM modes, we obtain two different eigenproblems. The propagation constant k_z plays the role of an eigenvalue, and the resulting $E_y(x)$ or $B_y(x)$ are eigenfunctions.

$$\text{TE:} \quad \partial_x^2 E_y + \frac{\omega^2 \varepsilon(x)}{c^2} E_y = k_z^2 E_y, \quad (6.10)$$

$$\text{TM:} \quad \partial_x \left(\frac{1}{\varepsilon(x)} \partial_x B_y \right) + \frac{\omega^2}{c^2} B_y = \frac{k_z^2}{\varepsilon(x)} B_y.$$

By solving these equations, we will obtain the dispersion curve $k_z(\omega)$.

There are many ways to find the dispersion curve. In this work, we will focus on the straightforward approach. After discretizing the space with the step Δx , we have a set of linear equations for the TE modes

$$\text{TE:} \quad \frac{E_y^{i+1} - 2E_y^i + E_y^{i-1}}{\Delta x^2} + \frac{\omega^2 \varepsilon(x_i)}{c^2} E_y^i = k_z^2 E_y^i. \quad (6.11)$$

We can rewrite this equation in matrix form and solve it, using standard solvers. Other components of the fields appear to be found from (6.9) as

$$\begin{aligned} \text{TM:} \quad E_x &= \frac{c^2 k_z}{\varepsilon \omega} B_y & \text{and} \quad \text{TE:} \quad B_x &= -\frac{k_z}{\omega} E_y \\ E_z &= \frac{i c^2}{\varepsilon \omega} \partial_x B_y & B_z &= \frac{1}{i \omega} \partial_x E_y \end{aligned} \quad (6.12)$$

For reference, for a symmetric waveguide with $\varepsilon_1 = \varepsilon_2 = 1$ and $\varepsilon_2 = 16$, the dispersion curves for TE and TM modes are shown in Fig. 6.3.

6.4 Assignments

1. Consider a symmetrical waveguide. Find the dispersion curves $k_z(\omega)$ for the TE and TM modes.
2. Compare the ray approximation (6.5) with the rigorous solution. Explain the differences.
3. Find the field distributions for the first few different modes.
4. Consider an asymmetric waveguide. Which features are the same as with the symmetrical one? Which features are different?

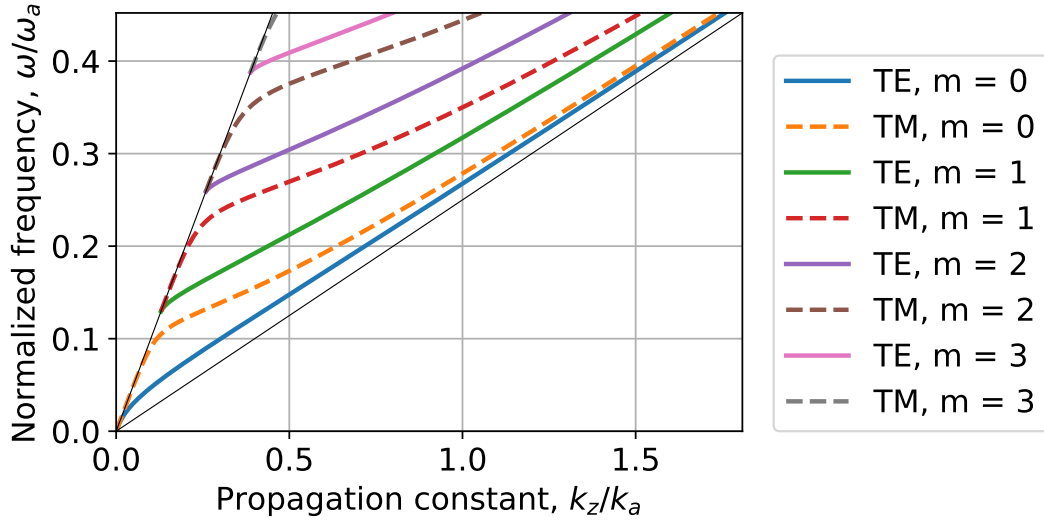


Figure 6.3: Dispersion of a symmetric dielectric planar waveguide. All the solutions are located between two the light cones (light in the surrounding medium and light in the medium of the guided region). The permittivities are $\varepsilon_1 = \varepsilon_3 = 1$, $\varepsilon_2 = 16$. The values are normalized to $k_a = 2\pi/a$ and $\omega_a = k_a c$.

6.5 References

The waveguide theory is a very broad and important field of science, as it has a huge number of practical applications such as optical waveguides for the Internet connection. There are many great books on this topic, to name just a few, please consult:

1. Okamoto, Katsunari. Fundamentals of optical waveguides. Academic press, 2006.
2. Chen, Chin-Lin. Foundations for guided-wave optics. John Wiley & Sons, 2006.
3. Snyder, Allan W., and John Love. Optical waveguide theory. Springer Science & Business Media, 2012.