PHOT 301: Quantum Photonics

Project topics: project 2

Michaël Barbier, Fall semester (2024-2025)

Introduction

There are four projects to be performed during the PHOT 301 course of this semester. This file contains the project topics for the second project. The projects are meant to focus more on applied "real world" problems.

You can and are encouraged to work together on projects, further, you can ask help from me and Yağız (asking help will not influence your project grade). However, your project report and any figures containing plots and/or schematics should be made individually and not copied from others or online resources. Please cite any sources that you used and where you used them (you don't have to cite this document).

Type of report for project 2

The report should be between one and two pages (one sheet) including figures. Please ask help to your instructors on time, we might have not enough time to help you at the last day before the deadline of the report.

Grading of the project

This project will count for 10% of your grade. During this semester four projects will be made in total, corresponding to 40% of your total grade.

Project topics

Next is a list of problems out of which you can choose for your project together with their task description. You only have to solve one problem for your project. Please inform me if the problem description contains any errors or anything is unclear.

You can use the code snippets in the separate document: `phot301_guidelines_for_the_projects.pdf` to construct any numerical methods required for your problem: transfer matrix method, finite basis method, tight-binding method, etc. There are also some code snippets provided for creating visualizations/plots. The code snippets are in Python, please inform me if you need help within another program (such as MATLAB).

Problem 1: Impact of the potential barrier shape on resonances in transmission and reflection

The transfer matrix method is a great method because it gives exact solutions for the wave function (given by simple propagating waves in each region of constant potential). When the approximation of the potential energy function $V(x)$ is not accurate, then it can lead to artifacts though. Here we consider the impact of the barrier shape on the transmission of a particle incident onto the barrier. See also page 45 in [1].

The transmission through a *single* 1D finite barrier with potential V inside the barrier exhibits various resonance peaks for energies $E > V$. When the barrier is smooth, these resonances should disappear.

- Compute and compare the transmission coefficient T of a square barrier with a Gaussian shaped barrier $V(x) \propto \exp\left(-x^2/(2\sigma)\right)$ by approximating the smooth barrier via the transfer matrix method.
- Stepwise increase the smoothness of the "smooth" barrier by increasing the step-wise pieces: I suggest comparing a barrier with a height of 1 eV and $\sigma = 1$ nm built-up from 1 (square barrier), 3, 7, and 15 pieces (see the figure below).
- Plot the transmission for these increasingly "smooth" barriers to show how resonances in the transmission slowly disappear.

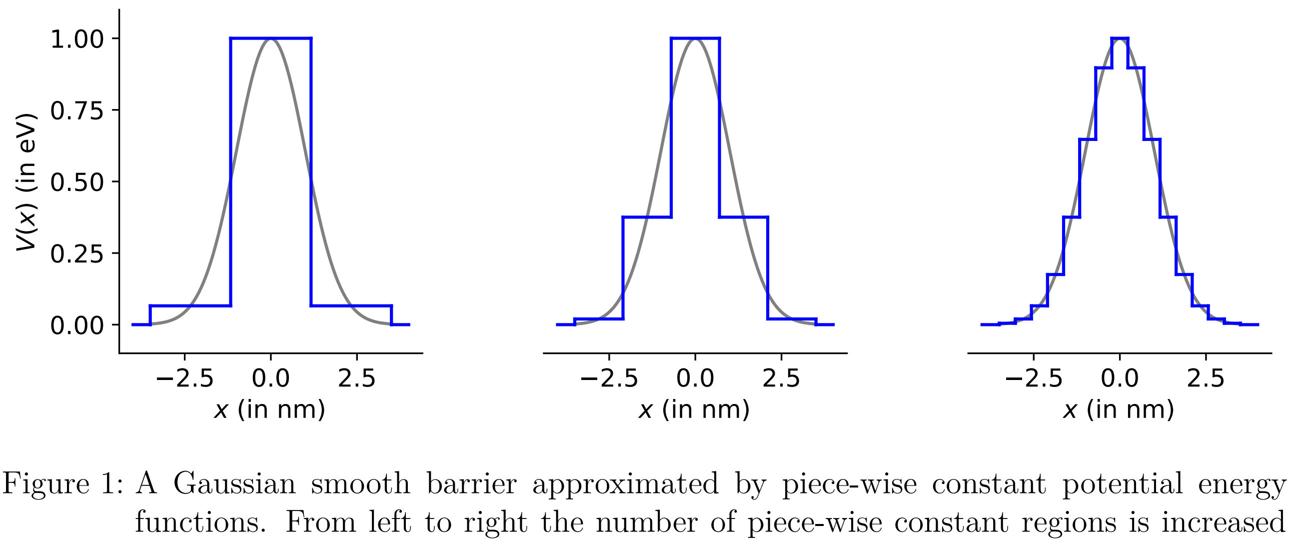

Figure 1: A Gaussian smooth barrier approximated by piece-wise constant potential energy functions. From left to right the number of piece-wise constant regions is increased resulting in better approximations of the Gaussian barrier: the barriers consists of 3, 5, and 15 parts respectively. The barrier region is defined within an interval of 3 standard deviations.

Problem 2: Bound states and transmission resonances in a double barrier system

In optical systems, gratings can be used as filters for specific wave lengths. In nanoscale systems, similarly, a series of potential barriers can serve the same purpose. Here we will consider the simplest *grating* possible: a double barrier.

The manner in which energies (corresponding to frequencies) that can pass are "chosen" can be understood as resonances in the transmission. To find the resonances we can look at the bound states of the *well* between the barriers (if we would assume the barriers would be very thick). These energy values of bound states in the well of a double barrier system correspond to the resonances in the transmission. The particles tunnel via the *quasi-bound states*, for a more detailed description see also page 288 of Miller's book [2].

- Compute the transmission for a double barrier system with inter-barrier distance of $L = 2$ nm, and for multiple barrier ticknesses $W = 0.25, 0.5, 1$ nm and constant barrier height of 0.25 eV.
- Then compute the bound states for a well with corresponding width, i.e., also equal to $L = 2$ nm and finite height of 0.25 eV (you can use the same transfer method method for that as well). Can you find transmission resonances (peaks in transmission), for similar energies?
- Plot and visually compare the transmission resonances for various thicknesses of the barriers. Show the impact of the barrier thickness on total transmission and sharpness of the transmission resonances.
- What parameter would you need to change if you want to optimize the system to work as a filter for a specific frequency(energy)? How do you get that energy to correspond to a transmission resonance? Which parameter do you need to change to optimize the sharpness of resonance peaks?

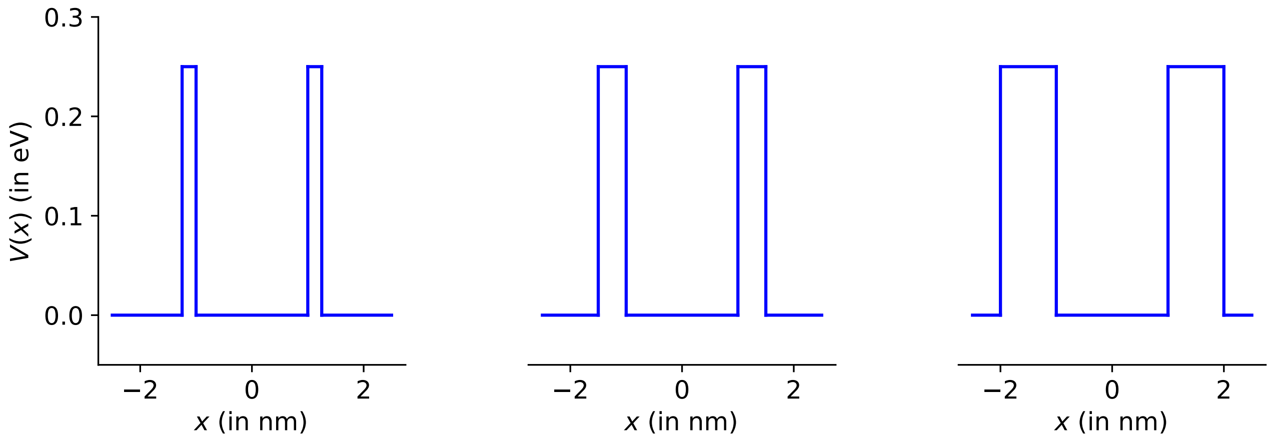

Figure 2: A 1D double potential barrier system with rectangular potential barrier with height of 0.25 eV and separated by 2 nm. The width of the barriers is increased from left to right and is equal to 0.25, 0.5, and 1 nm, respectively.

Problem 3: Free particle wave packets

Quantum mechanical wave packets propagating within a simple 1D system with constant potential $V(x)$ (as *free particles*) disperse in time, see also page 67 in Miller's book [2]. This is because a wave packet is a superposition of wave solutions e^{ikx} with different momentum, traveling at different velocities. Suppose a wave packet is defined by:

$$A(x,t) = \frac{\sqrt{\hbar}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i(kx-\omega(k)\,t)}\, dk$$

with the dispersion relation $\omega(k) = E(k)/\hbar$ telling us how the energy E of a wave component depends on the wave vector k. If $\omega(k) = \omega$ is a constant then the wave packet moves at a constant velocity without changing its shape since it becomes a function of $x - v\,t$ with the velocity $v = v_g = v_p = \frac{\omega}{k}$:

$$A(x,t) = \frac{\sqrt{\hbar}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ik(x-\frac{\omega}{k}t)}\, dk$$

If $\omega(k)$ is not a constant the group velocity v_g of the wave packet is proportional to the derivative of the energy to the momentum $v_g \propto \frac{d\omega}{dk}$. This we can see from expanding $\omega(k)$ around some fixed k_0:

$$\begin{aligned}
\omega(k) &= \omega(k_0) + (k-k_0)\left.\frac{d\omega}{dk}\right|_{k_0} + \frac{1}{2}\,(k-k_0)^2 \left.\frac{d^2\omega}{dk^2}\right|_{k_0} + ... \\
&= k_0 v_p + (k-k_0) v_g + \frac{1}{2}\,(k-k_0)^2\,\Gamma + ...
\end{aligned}$$

Here $v_p = \frac{\omega(k_0)}{k}$ is the phase velocity, $v_g = \left.\frac{d\omega}{dk}\right|_{k_0}$ is the group velocity as we saw before, and we defined a new parameter $\Gamma = \left.\frac{d^2\omega}{dk^2}\right|_{k_0}$.

Filling in this expression within the Gaussian wave packet we can write it in the following form (after some algebra):

$$\frac{\sqrt{\hbar}}{\sqrt{2\pi}\sigma(t)} \exp\left\{ -\frac{1}{2} \left(\frac{x-(x_0+v_g t)}{\sigma(t)} \right)^2 \right\} e^{i\theta(x,t)}$$

with

$$\text{Phase:} \qquad \theta(x,t) = k_0\, x - k_0\, t\,(v_g - v_p) - \frac{\Gamma\, t}{\Gamma^2\, t^2 + \sigma_x^4}$$

$$\text{Width:} \qquad \sigma(t) = \sigma_x \sqrt{1 + \frac{\Gamma^2}{\sigma_x^4}\, t^2}$$

If we look at the envelope function, that is we ignore the phase factor $e^{i\theta(x,t)}$, then we see that the velocity of the envelope function is still given by the group velocity v_g. Moreover, the broadening of the envelope function in time given by $\sigma(t)$ is determined by the Γ parameter. For a free particle with mass m we have $\omega(k) = E/\hbar = \frac{\hbar k^2}{2m}$ and thus $\Gamma = \frac{d^2\omega(k_0)}{dk^2} = \hbar/m$.

Perform the following tasks to understand the evolution of the probability density function of free particles:

- Compute the evolution of a wave packet of an electron (1D) in time. Use an average energy $E = \hbar^2 k_0^2/2m = 1$ eV and initial packet width given by $\sigma(t = 0) = 1$ nm.
- Plot 3 snapshots of the wave packet at different time points: $t = 0$ fs (femtoseconds), 10 fs, and 20 fs, to illustrate that the wave packet broadens. Have a look at the PhET wave packet simulator, see the link in reference [3], to verify your results.
- Visualize the broadening as function of time for wave packets of particles with different mass terms (so different values for Γ).
- If two wave packets of equal width but unequal energy/velocity travel a certain distance, say 20 nm, which one broadened more at arrival? How can you see that from the formulas?

Problem 4: Coherent states

In a harmonic oscillator coherent states can be formed, see page 63 in Miller's book [2]. These coherent states minimize the uncertainty in momentum/space, and approximate the classical motion of the classical harmonic oscillator, that is, a localized wave packet (and corresponding probability density) is oscillating forth and back in the quadratic well, not losing its localized nature over time. This is very different from free particles for which an initially localized wave packet broadens over time.

A coherent state is identified by a complex number α that represents an eigenvalue of the annihilation operator (i.e. the lowering ladder operator): $\hat{a}_- |\alpha\rangle = \alpha |\alpha\rangle$). The state is given by the following superposition of energy eigenstates $|n\rangle$ of the harmonic oscillator:

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2} |n\rangle$$

Remember that the eigenstates of the Hamiltonian were given by:

$$\hat{H}|n\rangle = E_n|n\rangle, \quad \text{with} \quad \hat{H} = \left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)\hbar\omega$$

Perform the following tasks (similar to problem 3.42 in Griffith's book [4]):

- Plot the contributions $|c_n|^2$ of each eigenstate $|n\rangle$, for different values of $|\alpha| = 5$, 10, and 20 (the phase doesn't matter here). What is the difference between states with smaller and larger values of $|\alpha|$?
- Plot how the expectation value of the energy $\langle \hat{H} \rangle$ varies as function of the magnitude $|\alpha|$.
- Prove that the eigenvalue α evolves in time as $\alpha(t) = \alpha\, e^{-i\omega t}$. Show this by adding the time-dependent factor to the eigenstates $|n\rangle \to \exp(-iE_n t/\hbar)\,|n\rangle$ with $E_n = (n+1/2)\hbar\omega$

- Calculate the evolution in time of the expectation values $\langle \hat{x} \rangle$, $\langle \hat{x}^2 \rangle$, $\langle \hat{p} \rangle$, and $\langle \hat{p}^2 \rangle$. Compare them with the classical harmonic oscillator.
- Use the expectation values calculated above to compare with the classical concept of a particle in a parabolic well. Show the following: The wave packet turns back at the classical *turning* points, see the figure below. The kinetic energy $T = \frac{p^2}{2m}$ is zero at those points, and potential energy $V(x) = \frac{1}{2}m\omega^2 x^2$ is maximal and equal to the total energy $\langle \hat{H} \rangle$.
- The wave packet can keep its shape partially by the fact that the energy levels are multiples of a common factor. This makes that any superposition of eigenstates periodically returns to the same interference pattern, i.e. the same state (and thus the same shape). What do you expect would happen in an infinite well? And in a finite well?

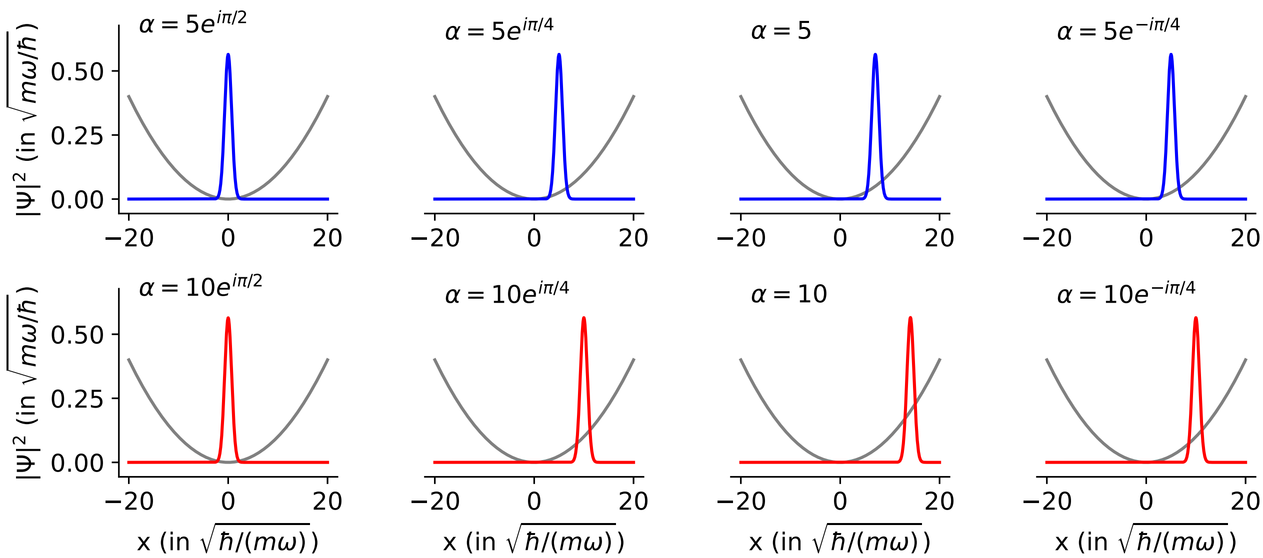

Figure 3: The evolution in time of the probability of a coherent state in a 1D quantum harmonic oscillator system. The upper (lower) plots show snapshots of the probability density function of a coherent state at multiple time points. The time points correspond to the alpha values given in the plots and the upper (lower) plots correspond to a magnitude of 5 (10) for alpha. The turning point (on the right) is reached in the 3rd panels from the left, after which the packet slowly return in the fourth panels from the left.

References

[1] Robert Gilmore, *Elementary Quantum Mechanics in One Dimension*, Baltimore, Maryland, USA: The John Hopkins University Press, 2004.

[2] David A. B. Miller, *Quantum Mechanics for Scientists and Engineers*, Cambridge University Press, USA, 2008.

[3] Quantum Tunneling and Wave Packets, A wave packet simulator that is part of the collection of PhET Interactive Simulations of the University of Colorado.

[4] David J. Griffiths, Darrell F. Schroeter, *Introduction to Quantum Mechanics*, 3rd Ed., Cambridge University Press, UK, 2018.