TFY4235/FY8904: Computational Physics (spring 2019)

# Assignment 2: The World of Quantum Mechanics

Mohammad Alidoust, Arnau Sala and Ingve Simonsen

Department of Physics, NTNU – Norwegian University of Science and Technology, Trondheim

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**Abstract**

In this assignment we will study three different quantum mechanical systems, described by one-dimensional Schrödinger equations. The first problem is the simple and well-known particle in a box, where we focus on scaling to dimensionless equations and comparing computational results to the exact ones. The second problem describes a particle in a box with a potential barrier, where we do not have many analytical results. It is perfect for testing intuitive understanding of a problem, and for asking the ultimate questions in computational physics: Do my results make sense? Why do I think they should? In the third problem we learn how we can study a simple time-dependent quantum mechanical platform. By considering a time-dependent Schrödinger equation for oscillating adjacent quantum wells we find a time-dependent wavefunction that result in an integral equation. Finding the time-dependent wavefunction, we predict the evolution of non-interacting particles that might exist in this system.

**Relevant fields**: Quantum mechanics.

**Mathematical and numerical methods**: Linear algebra, scaling to dimensionless units, using complex numbers, root-finding, PDEs, finite difference, numerical integration, integral equation.

**Contact**: mohammad.alidoust@ntnu.no; arnau.sala@ntnu.no; ingve.simonsen@ntnu.no

# 1 Introduction

Quantum mechanics (QM) is an extensive field that is used for a wide variety of physics (and chemistry). Technologies like lasers, light-emitting diodes (LEDs), magnetic resonance imaging (MRI), and electron microscopy are all based on quantum mechanical effects. Through earlier courses you might be familiar with the principles of quantum mechanics and how to solve problems analytically, but numerics is often neglected. However, there are a lot of problems that we have to solve numerically and they cannot be solved analytically. We will not spend too much time solving problems that are not analytically solvable, but instead focus on issues that can arise when we try to solve quantum mechanical problems numerically.

Still, keep in mind throughout this assignment that computational QM is an important field in itself, not just something we do to compare results with readily available analytical solutions.

Exact solutions are, however, very useful for testing your code.

Tasks preceded by ($\star$) require some mathematical analysis. Although you can skip them and go straight to the numerics, we encourage you to work on these problems to gain a better understanding of the problem at hand.

# 2 Particle in a box and dimensionless variables

## 2.1 The Schrödinger equation

The Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi, \tag{2.1}$$

is the baseline of quantum mechanics, and describes how a system evolves in time given the Hamiltonian operator $\hat{H}$ for the system. The evolution of the wave function $\Psi$ in time and space is given by Eq. (2.1), where $\Psi$ depends on time and the spatial coordinates of the system. (For a single particle in 1D this means that $\Psi = \Psi(x,t)$.) The wave function contains all available information about the system at hand. Equation (2.1) can in principle describe any system, but for complicated systems it is often difficult both to construct the correct Hamiltonian and to actually solve the equation once the appropriate Hamiltonian has been found.

Given an initial condition $\Psi_0(x) = \Psi(x, t = 0)$ and a time-independent Hamiltonian, the Schrödinger equation has a formal solution

$$\Psi = \exp\left(-\frac{it}{\hbar}\hat{H}\right)\Psi_0, \tag{2.2}$$

where the exponential of the Hamiltonian operator is given by its series expansion. This equation formally describes the evolution of the system in time, but it is not that useful unless we know the eigenfunctions – often called eigenstates in QM – $\psi_n$ of the Hamiltonian. They are given by the time-independent Schrödinger equation

$$\hat{H}\psi_n = E_n\psi_n, \tag{2.3}$$

where $E_n$ is the energy of the state $\psi_n$. Hence the Hamiltonian is often known as the energy operator. The Hamiltonian is the only thing (!) that makes Eq. (2.1) different, for instance, when applying it to a particle in a 1D box and an interacting electron gas in 3D. So to investigate a certain system, we first need to find its Hamiltonian.

## 2.2 The Hamiltonian

We want to study a single particle with mass $m$ confined in a 1D box with walls at $x = 0, L$.

**Task 2.1:** What are boundary conditions for the wave function $\Psi(x,t)$ when the particle is confined in this box? (Hint: Remember that $|\Psi(x,t)|^2$ is the probability density of the particle at time $t$ and that $\Psi$ must be continuous as a function of $x$.)

The potential that describes this box is

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{otherwise.} \end{cases} \tag{2.4}$$

From this we can construct the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x), \tag{2.5}$$

which means that Eqs. (2.1) and (2.3), the time-dependent and time-independent Schrödinger equations, read

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = i\hbar\frac{\partial}{\partial t}\Psi \tag{2.6}$$

and

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2} = E_n\psi_n \tag{2.7}$$

inside the box. (Since $V(x) = 0$ inside the box.)

## 2.3 Dimensionless variables

To actually solve these equations we cannot immediately start implementing numerical algorithms. First we must make the equations dimensionless, as number representations on your computer do not contain any physical units. (Although a few programming languages can keep track of units for you.)

**Task 2.2:** ($\star$) Define new dimensionless variables $t' = t/t_0$ and $x' = x/x_0$. The values $t_0$ and $x_0$ are the scales that time and position is measured in with the new coordinates $t'$ and $x'$. These scales can be chosen arbitrarily, but some values are easier to work with than others. Show that by choosing $x_0 = L$ and an appropriate value for $t_0$, Eq. (2.6) can be written

$$i\frac{\partial\Psi}{\partial t'} = -\frac{\partial^2\Psi}{\partial x'^2}. \tag{2.8}$$

(Hint: Use the chain rule for differentiation on $\Psi(x, t'(t))$ to find a relation between $\frac{\partial\Psi}{\partial t}$ and $\frac{\partial\Psi}{\partial t'}$. You can do the same thing with $x$ and $x'$.)

**Task 2.3:** ($\star$) With the new variables $t'$ and $x'$, show that Eq. (2.7) can be written

$$-\frac{\partial^2\psi_n}{\partial x'^2} = \lambda_n\psi_n, \tag{2.9}$$

and find the relation between $\lambda_n$ and energy $E_n$.

**Task 2.4:** Now that we have changed our variables, remember that the boundary conditions have also changed. What are the boundary conditions in the new variables? Why do you think we chose $x_0 = L$? Could we have chosen other values of $x_0$ instead?

## 2.4 Eigenvalues and eigenfunctions

Now that we have finally found a set of equations with dimensionless variables we can get to work by solving the problem at hand.

**Task 2.4:** Discretize the position $x'$ inside the box. Then apply a finite difference scheme on Eq. (2.9) and solve the emerging matrix problem.

We now have a list of eigenvalues $\lambda_n$ and corresponding eigenfunctions $\psi_n$. If we have used a small discretization step $\Delta x'$ it can be useful to store these values in a file for later use instead of calculating them all over again the next time we run our program.

**Bonus task:** ($\star$) Show that the exact (and properly normalized) solution of Eq. (2.9) is given by

$$\psi_n(x') = \sqrt{2}\sin(n\pi x') \tag{2.10}$$

for $n = 1, 2, 3, \ldots$ with corresponding eigenvalues $\lambda_n = (\pi n)^2$.

**Task 2.5:** Plot your computed energy eigenvalues against $\lambda_n = (\pi n)^2$, the energies of the exact eigenstates in Eq. (2.10). Remember to use the axis label of your plot to specify on what scale the energies are. Otherwise the values are meaningless to other people, who might have used different values of $t_0$ and $x_0$. (Hint: You are plotting $\lambda_n$ as a function of $n$. The axis label should then contain the expression $\lambda_n(E_n)$. It should look like $E_n/E_0$ where $E_0$ is the relation between $\lambda_n$ and $E_n$ that you found in Task 2.3.)

**Task 2.6:** Now compare your eigenfunctions to the ones in Eq. (2.10). Introduce a measure of error between them and investigate how it scales with the discretization step $\Delta x'$.

## 2.5 Expansion in eigenfunctions

If we know the expansion of the initial condition $\Psi_0$ in the eigenfunctions $\psi_n$,

$$\Psi_0(x) = \sum_n \alpha_n \psi_n(x), \tag{2.11}$$

then Eq. (2.2) immediately gives us the time evolution of the system

$$\Psi(x,t) = \exp\left(-\frac{it}{\hbar}\hat{H}\right)\Psi_0(x) = \sum_n \alpha_n \exp\left(-\frac{iE_n t}{\hbar}\right)\psi_n(x). \tag{2.12}$$

**Task 2.7:** ($\star$) Show that the dimensionless version of Eq. (2.12) reads

$$\Psi(x',t') = \sum_n \alpha_n \exp\left(-i\lambda_n t'\right)\psi_n(x'). \tag{2.13}$$

With Eqs. (2.11) and (2.13) in place, we can find the state $\Psi(x',t')$ of the system at any time $t'$ when the initial condition $\Psi(x',0) = \Psi_0(x')$ is given. To use these equations we first need the coefficients $\alpha_n$ from Eq. (2.11), which we can calculate using the inner product between the initial state $\Psi_0$ and the eigenstates $\psi_n$,

$$\alpha_n = \langle \psi_n, \Psi_0 \rangle = \int \psi_n^*(x')\Psi_0(x')\mathrm{d}x', \tag{2.14}$$

where $\psi^*$ means the complex conjugate of $\psi$. In this case the eigenfunctions are real, as shown in Eq. (2.10).

**Task 2.8:** Write a code that can solve the integral in Eq. (2.14) numerically.

The eigenstates $\psi_n$ of the Hamiltonian are orthogonal when they have different eigenvalues, i.e. they satisfy $\langle \psi_n, \psi_m \rangle = \delta_{n,m}$, so for $n \neq m$ the inner product is zero.

**Task 2.9:** Check the orthogonality of your computed eigenstates using your code from Task 2.8.

## 2.6 Initial conditions and solutions

Now that all the necessary machinery is ready, let us try to solve the Schrödinger equation for the particle in a box. We first need to specify an initial condition.

**Task 2.10:** First test your code for the initial condition $\Psi_0(x') = \sqrt{2}\sin(\pi x')$, the first eigenfunction from the exact solution. Use Eq. (2.14) to calculate the coefficients $\alpha_n$ and then Eq. (2.13) to find the state of the system at a time $t' > 0$. Do you get the expected results? Is the wave function $\Psi(x',t')$ correctly normalized? (Hint: Remember that $|\Psi(x',t')|^2$ is the probability density of the particle at time $t'$. Hence it should satisfy the condition

$\int |\Psi(x',t')|^2 \mathrm{d}x' = 1$.)

**Task 2.11:** Now try to use a delta function as initial condition, $\Psi_0(x') = \delta(x' - 1/2)$. Do you think your results for $t' > 0$ are correct? Why or why not? (Hint: Look at what happens with Eq. (2.14).)

# 3 Box with a potential barrier

We will now look at a similar problem, but with a twist. This time the particle is still confined in a box on the interval $[0, L]$, but the middle third of the box contains a potential barrier with a strength $V_0$

$$V(x) = \begin{cases} 0 & \text{for} \quad 0 < x < \frac{L}{3} \\ V_0 & \text{for} \quad \frac{L}{3} < x < \frac{2L}{3} \\ 0 & \text{for} \quad \frac{2L}{3} < x < L \\ \infty & \text{otherwise.} \end{cases} \tag{3.1}$$

To solve this problem numerically we create the dimensionless variables $t' = t/t_0$ and $x' = x/x_0$ with the same choices of $t_0$ and $x_0$ as in Task 2.2. This gives us the dimensionless Schrödinger equation

$$i\frac{\partial \Psi}{\partial t'}(x',t') = \left[-\frac{\partial^2}{\partial x'^2} + \nu(x')\right]\Psi(x',t'), \tag{3.2}$$

where $\nu(x) = t_0 V(x)/\hbar$. Let's also define $\nu_0 = t_0 V_0/\hbar$ as a dimensionless measure of the strength of the potential barrier. The corresponding time-independent Schrödinger equation becomes

$$\left[-\frac{\partial^2}{\partial x'^2} + \nu(x')\right]\psi_n(x') = \lambda_n \psi_n(x'), \tag{3.3}$$

with $\lambda_n$ related to the energy eigenvalues $E_n$ as in the earlier tasks.

**Task 3.1:** Discretize the dimensionless Hamiltonian, the expression in the square brackets on the left-hand side of Eq. (3.3). Choose $\nu_0 = 0$ and solve the equation for the eigenvalues and eigenvectors. Does this match your results from Task 2.4?

## 3.1 A high barrier

Let the barrier constant $\nu_0$ take a fairly large value, for instance $\nu_0 = 10^3$.

**Task 3.2:** Find the eigenvalues and corresponding eigenvectors of the Hamiltonian for this system, then plot the first few eigenvectors and take a look at their eigenvalues. Do you notice anything strange? Why do you think the results look like this? (Hint: A one-dimensional problem like this cannot have degenerate bound states. See e.g. section 3.1.3 in Ref [1] for an explanation in Norwegian.)

**Task 3.3:** Let the initial condition be the superposition of the two first eigenstates from Eq. (3.3), $\Psi_0 = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$, which is mainly localized on one side of the barrier. Use Eqs. (2.13) and (2.14) to evolve the system to a time $t' = \pi/(\lambda_2 - \lambda_1)$. What happens and why does it happen at this particular time? How does the probability density $|\Psi(x',t')|^2$ behave between $t' = 0$ and $t' = \pi/(\lambda_2 - \lambda_1)$?

This is an example of quantum tunnelling, where the particle — or, rather, its probability density — moves from one side of the barrier to the other, even though its possible energies, $\lambda_1$ and $\lambda_2$, are lower than the barrier $\nu_0$.

**Bonus task:** Use the initial condition from Task 3.3 and find the probability density of the particle, $|\Psi(x', t')|^2$, at evenly distributed later times $t'$. Then make an animation to show how it evolves in time.

## 3.2 Root-finding

You might have noticed that for $\nu_0 = 10^3$ there are several eigenvectors $\psi_n$ with energies $\lambda_n < \nu_0$. But how many are there and how accurately have we found these energies? And how does this depend on the value of $\nu_0$? To answer some of these questions we will need a little help from exact results and root-finding. We can show that eigenvectors of the Hamiltonian with energies $0 < \lambda < \nu_0$ are given by the equation[1]

$$f(\lambda) = \mathrm{e}^{\kappa/3}\left[\kappa \sin\left(\frac{k}{3}\right) + k\cos\left(\frac{k}{3}\right)\right]^2 - \mathrm{e}^{-\kappa/3}\left[\kappa \sin\left(\frac{k}{3}\right) - k\cos\left(\frac{k}{3}\right)\right]^2 = 0, \tag{3.4}$$

where we have defined $k = \sqrt{\lambda}$ and $\kappa = \sqrt{\nu_0 - \lambda}$ to somewhat simplify the expression.

In general, finding the roots of a function is a non-trivial procedure, and there is no way to guarantee that you have found all the roots of your function. Multiple roots or very close roots can, in particular, be difficult to detect. (If you want to read about root-finding and several different algorithms, take a look at Chapter 9 in Ref. [2].) Fortunately for us, we have a lot of information at our disposal. We have an analytical expression for $f(\lambda)$ and some good ideas about where its zeros are from the eigenvalues we computed earlier.

**Task 3.4:** Plot $f(\lambda)$ from Eq. (3.4) to get an idea of what it looks like. Are the zeros placed like you expected them to be from the earlier computation of the eigenvalues?

**Task 3.5:** Write a root-finding algorithm that solves Eq. (3.4). Remember to make use of the information at your disposal, i.e. the eigenvalues you computed earlier and the shape of $f(\lambda)$ from your plot. Then compare the energies to the ones you found in Task 3.2. (Hint: You can use a minimization function to separate roots that are very close to each other.)

**Task 3.6:** Investigate different values of the barrier height. How does the number of eigenstates with $\lambda_n < \nu_0$ depend on $\nu_0$? Try to estimate the value that separates having one and no such states.

**Bonus task:** Find analytically the value of $\nu_0$ that separates having a ground state $\psi_0$ with $\lambda_0 < \nu_0$ and having a ground state with $\lambda_0 > \nu_0$.

## 3.3 Step-by-step time evolution

So far we have used the eigenstates of the Hamiltonian to find the time evolution of the system by projecting the initial condition on the set of eigenstates[2]. But there are other ways to do this as well. For two times separated by $\Delta t'$ we can write the formal solution of the Schrödinger equation, Eq. (2.2), as

[1] I do not have a reference for this where you can look up the derivation. However, Eq. (3.4) is more tedious than difficult to derive, so you should be able to do it yourselves.

[2] For a time-dependent Hamiltonian this method doesn't work, meaning that we have to solve the Schrödinger equation in some other way.

$$\Psi(x', t' + \Delta t') = \exp\left(-i\Delta t' \hat{H}'\right) \Psi(x', t'), \tag{3.5}$$

where $\hat{H}'$ is the dimensionless Hamiltonian operator from Eq. (3.3). If $\Delta t'$ is sufficiently small the exponential can be approximated by the first few terms in a series expansion. This gives us a matrix problem that we can solve for $\Psi(x', t' + \Delta t')$ given $\Psi(x', t')$.

Let us first use the approximation $\exp(-i\Delta t' \hat{H}') \approx 1 - i\Delta t' \hat{H}'$. It gives us the matrix problem

$$\Psi(x', t' + \Delta t') = \left[1 - i\Delta t' \hat{H}'\right] \Psi(x', t'), \tag{3.6}$$

which you might recognize as the forward Euler scheme for the dimensionless Schrödinger equation.

**Task 3.7:** Use Eq. (3.6) to solve the Schrödinger equation with the initial condition $\Psi_0(x) = \psi_1(x)$, the ground state you found numerically in Task 3.2. What happens when enough time steps are taken? Does this depend on the Courant-Friedrichs-Lewy (CFL) number $\Delta t/\Delta x^2$?

The lesson from this task should be that we cannot pick a discretization scheme arbitrarily and expect it to work. The Schrödinger equation preserves probabilities, but the forward Euler scheme in Eq. (3.6) does not. To make a scheme that is consistent with conservation of probability we need our approximation of the time evolution operator, $\exp(-i\Delta t' \hat{H}')$, to be unitary.

A quantum mechanical operator $\hat{A}$ is unitary if its adjoint $\hat{A}^\dagger$ is its inverse, i.e. $\hat{A}\hat{A}^\dagger = \hat{A}^\dagger\hat{A} = I$. This is satisfied by the time evolution operator $\exp(-i\Delta t' \hat{H}')$ since the Hamiltonian is self-adjoint ($\hat{H}^\dagger = \hat{H}$). As a unitary approximation we can choose

$$\exp\left(-i\Delta t' \hat{H}'\right) \approx \frac{1 - \frac{i}{2}\Delta t' \hat{H}'}{1 + \frac{i}{2}\Delta t' \hat{H}'}, \tag{3.7}$$

where division with an operator means multiplication with its inverse. This gives us

$$\left[1 + \frac{i}{2}\Delta t' \hat{H}'\right] \Psi(x', t' + \Delta t') = \left[1 - \frac{i}{2}\Delta t' \hat{H}'\right] \Psi(x', t'), \tag{3.8}$$

which is easily recognizable as the Crank-Nicolson scheme by rearranging the terms.

**Task 3.8:** Think about when this method of step-by-step time evolution is advantageous compared to the expansion in eigenstates that we did earlier. Does it depend on the initial condition? Make a few hypotheses.

**Task 3.9:** Test your ideas from Task 3.8 by using the Crank-Nicolson scheme from Eq. (3.8).

# 4 Periodic detuning of a two-level system

We have seen that the two lowest energy levels are very close in energy but very far away from all the others. If we focus on the low energy regime then the double well can be considered as a two-level system, in analogy to a double quantum dot charge qubit [3]. In this section we are going to construct an effective Hamiltonian that reproduces the dynamics of the double well in the low-energy regime. We are then going to detune the two-level system with a periodic, time-dependent potential to enforce a population transfer from one quantum state to the other.

## 4.1 A lower barrier

In the last section we used a time-independent potential with a very high barrier. Now we need to reduce the height of the barrier to allow for easier tunneling events. Consider the following time-dependent potential:

$$V(x,t) = \begin{cases} 0 & \text{for} \quad 0 < x < \frac{L}{3} \\ V_0 & \text{for} \quad \frac{L}{3} < x < \frac{2L}{3} \\ V_r(t) & \text{for} \quad \frac{2L}{3} < x < L \\ \infty & \text{otherwise,} \end{cases} \tag{4.1}$$

**Task 4.1:** Set $\nu_0 = 100$ (recall that $\nu(x,t) = t_0 V(x,t)/\hbar$) and plot the two lowest eigenvalues as a function of $V_r$ (or rather $\nu_r$). For this exercise we don't need to know the explicit time dependence of $V_r$, so let's just write $V(x, V_r)$ and let $V_r$ take both positive and negative numbers.

You can check that for very large $V_r$, the ground state is mostly localized on the left of the barrier, while for negative $V_r$, the ground state is on the other side. Measure also the energy difference $\varepsilon_0$ between the ground state and the excited state at zero detuning, that is, for $V_r = 0$.

## 4.2 An effective two-level system

At zero detuning the energy $\varepsilon_0$ is minimum, and as we increase or decrease the potential on the right side the energy difference increases. Such a system can be modeled by a very simple $2 \times 2$ Hamiltonian:

$$\hat{H}_{\text{eff}} = \begin{pmatrix} -\varepsilon_0/2 & \tau \\ \tau & \varepsilon_0/2 \end{pmatrix}, \tag{4.2}$$

where the tunneling amplitude $\tau$ is a function of $\nu_r$ and we have shifted the total energy of the system to make the Hamiltonian traceless. This simplifies the analytical calculations. The next step consists on finding $\tau(\nu_r)$.

Suppose we prepare the system in the state $|g_0\rangle$, the ground state at $\nu_r = 0$. This state has an energy $-\varepsilon_0/2$. Consider also the state $|e_0\rangle$, the excited state at $\nu_r = 0$, with energy $\varepsilon_0/2$. The tunneling amplitude is then

$$\begin{aligned} \tau &= \langle g_0 | \hat{H} | e_0 \rangle \\ &= \int_0^L dx'\, \psi_0(x') \left( -\frac{\partial^2}{\partial x'^2} + \nu(x', \nu_r) \right) \psi_1(x'). \end{aligned} \tag{4.3}$$

Note that for $\nu_r = 0$ the two eigenstates are orthogonal and the integral vanishes, but for $\nu_r \neq 0$, the tunneling amplitude is finite.

**Task 4.2:** Calculate this integral for different values of $\nu_r$ and find an expression for $\tau(\nu_r)$. With this we have checked the validity of the two-level Hamiltonian shown above. Now we have all the elements that we need to play with our effective two-level system.

## 4.3 Enforced quantum population transfer: Rabi oscillations

Interestingly, changing the potential offset of only one of the quantum wells yields a two-level system with a varying tunneling amplitude. This tunneling amplitude is the element that couples the two quantum states and now we shall see that when we are at zero detuning, a weak

modulation of the tunneling amplitude (i.e., the potential offset $V_r$) will enforce transitions from one quantum state to another if this modulation is in resonance with the energy splitting $\varepsilon_0$.

Consider now the Hamiltonian

$$\hat{H}_{\text{eff}} = \begin{pmatrix} -\varepsilon_0/2 & \tau \sin(\omega t) \\ \tau \sin(\omega t) & \varepsilon_0/2 \end{pmatrix}, \tag{4.4}$$

with $\tau$ very small compared with the energy splitting $\varepsilon_0$, such as $\tau = 0.02\varepsilon_0$. Since this Hamiltonian is time-dependent we cannot use the same methods we used before to find the time evolution of the states. To solve this system we are going to switch to the interaction picture.

In the interaction picture, the Schrödinger equation reads:

$$i\hbar \frac{d}{dt}|\psi(t)\rangle_I = \hat{H}_{1I}(t)|\psi(t)\rangle_I, \tag{4.5}$$

with $\hat{H}_{1I}(t)$ the interaction Hamiltonian in the interaction picture. Given a Hamiltonian $\hat{H}_{\text{eff}} = \hat{H}_0 + \hat{H}_1$, with

$$\hat{H}_0 = \begin{pmatrix} -\varepsilon_0/2 & 0 \\ 0 & \varepsilon_0/2 \end{pmatrix}, \tag{4.6}$$

$$\hat{H}_1 = \begin{pmatrix} 0 & \tau \sin(\omega t) \\ \tau \sin(\omega t) & 0 \end{pmatrix}, \tag{4.7}$$

the interaction Hamiltonian $\hat{H}_{1I}(t)$ reads

$$\hat{H}_{1I} = \begin{pmatrix} 0 & e^{-i\varepsilon_0 t/\hbar}\tau \sin(\omega t) \\ e^{i\varepsilon_0 t/\hbar}\tau \sin(\omega t) & 0 \end{pmatrix}. \tag{4.8}$$

The formal solution of the Schrödinger equation is then:

$$|\psi(t)\rangle_I = |\psi(0)\rangle - \frac{i}{\hbar}\int_0^t dt'\, \hat{H}_{1I}(t')|\psi(t')\rangle_I. \tag{4.9}$$

This is a Volterra integral equation that can be solved by discretizing the integral.

**Task 4.3:** Consider the state $|\psi(t)\rangle_I$ as an $n \times 2$ array, where each pair of elements contains $|\psi(t = k\,\Delta t)\rangle_I$ for $k \in \{0, n\}$. Write down the equation above for $|\psi(k\,\Delta t)\rangle_I$ discretizing the integral using the method that you consider most convenient. That is, transform the integral into a sum.

**Task 4.4:** If you have done this right now you have an equation of the form

$$\hat{\mathbf{M}}_k \cdot \mathbf{f}_k = \mathbf{f}_0 + \sum_{l=0}^{k-1} \hat{\mathbf{N}}_l \cdot \mathbf{f}_l, \tag{4.10}$$

with $\hat{\mathbf{M}}_k$ and $\hat{\mathbf{N}}_l$ being $2 \times 2$ matrices and $\mathbf{f}_k$ a two-components vector. Using $|\psi(0)\rangle = |g_0\rangle$ solve the integral equation for different $k$ from 1 to some $n$ by making use of an algorithm to

solve systems of linear equations. For this task you have to choose a frequency $\omega$. Use $\omega = \varepsilon_0$.

**Task 4.5:** Calculate the probability to find the system in the state $|e_0\rangle$ after a time $t$:

$$\begin{aligned} p(t) &= |{}_I\langle g_0|\psi(t)\rangle_I|^2 \\ &= |\langle g_0|\psi(t)\rangle_I|^2. \end{aligned} \tag{4.11}$$

**Task 4.6:** An approximate analytical solution to this problem can be found by switching to a rotating frame and then applying the so-called "rotating wave approximation", to average out the terms in the Hamiltonian that rotate very fast and keep only those that rotate very slowly. With this method, when the system is in resonance, i.e., $\omega = \varepsilon_0$, one can obtain the probability:

$$p(t) = \sin^2\left(\frac{t\tau}{2\hbar}\right). \tag{4.12}$$

Plot the analytical and numerical solutions together and check the validity of your results.

In this plot you should observe periodic oscillations from state $|g_0\rangle$ to $|e_0\rangle$. You should be surprised about these results. What you just found is that given a two-level system described by a Hamiltonian with a sinusoidal tunneling amplitude, you can enforce periodic transitions from one quantum state to the other with a frequency that is proportional to the amplitude of the detuning.

Check also what happens when the frequency of the detuning does not match the energy splitting of the two-level system $\varepsilon_0$. And what happens when $\tau$ is too large? Do you see the secondary oscillations in the probability?

# 5 Report

Write a report of your work (maximum 6 pages). The report is expected to take the form of a scientific article, containing an abstract, a short introduction, the modeling of the problem, a few words on its numerical resolution, your results and discussion, a conclusion and references. The tasks are here to guide you, and you should not write your answers task by task in the report, but rather select the important pieces of information showing in a concise way how you dealt with the problem, and critically discuss your results. Your codes are not expected in the report, but must be attached to it if it is delivered during the exam. Codes must be clear, and commented.

# References


[1] P. C. Hemmer. *Kvantemekanikk*. Tapir Akademiske Forlag, Trondheim, 5th edition, 2005.

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[3] J. Gorman, D. G. Hasko, and D. A. Williams. Charge-qubit operation of an isolated double quantum dot. *Phys. Rev. Lett.*, 95:090502, Aug 2005.