TFY4235/FY8904: Computational Physics (spring 2019) Assignment 2 – Shrödinger Equation

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Importance of Differential Equations (DE)

Ordinary Differential Equations (ODE)

Differential equations appear in numerous branches of Science and Engineering.
Most of the laws in physics and chemistry are differential equations!

Examples are:
1. Newton's law of motion (who invented the DEs independently of Gottfried Leibniz -1670-)

$$F = ma \rightarrow F = \frac{dv}{dt} = \frac{d^2x}{dt^2} \rightarrow \text{predicts the location of partilce} \quad (1)$$

2. Imagine we would like to simulate the growth pattern of bacterias in time. This can be simulated by the natural growth equation

$$\frac{dY(t)}{dt} = f(t)Y(t) \rightarrow \text{ simplest case} \rightarrow f(t) = f_0 = \text{ constant} \quad (2)$$

$$Y(t) = Y(t=0)e^{\pm|f_0|t} \quad (3)$$

Partial Differential Equations (PDE)

3. Maxwell's equations of the electromagnetic waves:
In the absence of electric charge and currents, such as in a vacuum, Maxwell's equations reduce to the following PDEs

$$\begin{cases} \mu_0\epsilon_0 \frac{\partial^2}{\partial t^2}\mathbf{E} - \boldsymbol{\nabla}^2\mathbf{E} = \mathbf{0}, \\ \\ \mu_0\epsilon_0 \frac{\partial^2}{\partial t^2}\mathbf{B} - \boldsymbol{\nabla}^2\mathbf{B} = \mathbf{0}, \end{cases} \rightarrow \boldsymbol{\nabla}^2 \equiv \left(\frac{\partial^2}{\partial_x^2}, \frac{\partial^2}{\partial_y^2}, \frac{\partial^2}{\partial_z^2}\right) \tag{4}$$

ODEs: involve functions with only one variable, say x.
PDEs: involve functions with more than one variable, say x, t.

Partial Differential Equations (PDE)

Last example:

4. Shrödinger equation, describing particles from a wave-like point of view.

$$-\boldsymbol{\nabla}^2\Psi(\mathbf{r},\mathbf{t}) + \mathrm{V}(\mathbf{r},\mathbf{t})\boldsymbol{\Psi}(\mathbf{r},\mathbf{t}) = \mathbf{i}\hbar\frac{\partial}{\partial \mathbf{t}}\boldsymbol{\Psi}(\mathbf{r},\mathbf{t}) \tag{5}$$

$\Psi(\mathbf{r},\mathbf{t})$: The wave function of particle as a function of location and time
$\mathrm{V}(\mathbf{r},\mathbf{t})$: The potential that the particle experiences
$\hbar = h/2\pi$: Planck's constant
E: The energy of particle

- In what follows, we deal with Linear PDEs. The nonlinear PDEs do not have unique solutions.
- In general, in order to solve a DE for specific situations, one needs to know initial conditions and boundary conditions.
  There are only few simple cases that result in analytical solutions and we might be able to obtain a general solution for a DE.

Solving 1D Shrödinger equation

Hamiltonian

Generally, in order to describe a physical system (involving moving particles, electric and magnetic fields, interactions etc.), one needs to construct a proper Hamiltonian (**H**) that has a dimension of energy — both in the Classical Mechanics and Quantum Mechanics
In this notation, the Shrödinger equation takes the following form:

$$\mathbf{H}(\mathbf{r}, t)\Psi(\mathbf{r}, t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) \tag{6}$$

Solving this PDE, in general, is a formidable task. However, let us make some simplifying assumptions.

Hamiltonian

Consider a situation where $H(\mathbf{r}, t) = H(\mathbf{r})$ is time-independent. The wavefunction should be a solution of the right hand side. An obvious solution is proportional to $\exp(-itE/\hbar)$ and the Shrödinger equation takes the following form

$$\mathbf{H}(\mathbf{r})\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \tag{7}$$

Particle in a perfect 1D quantum well

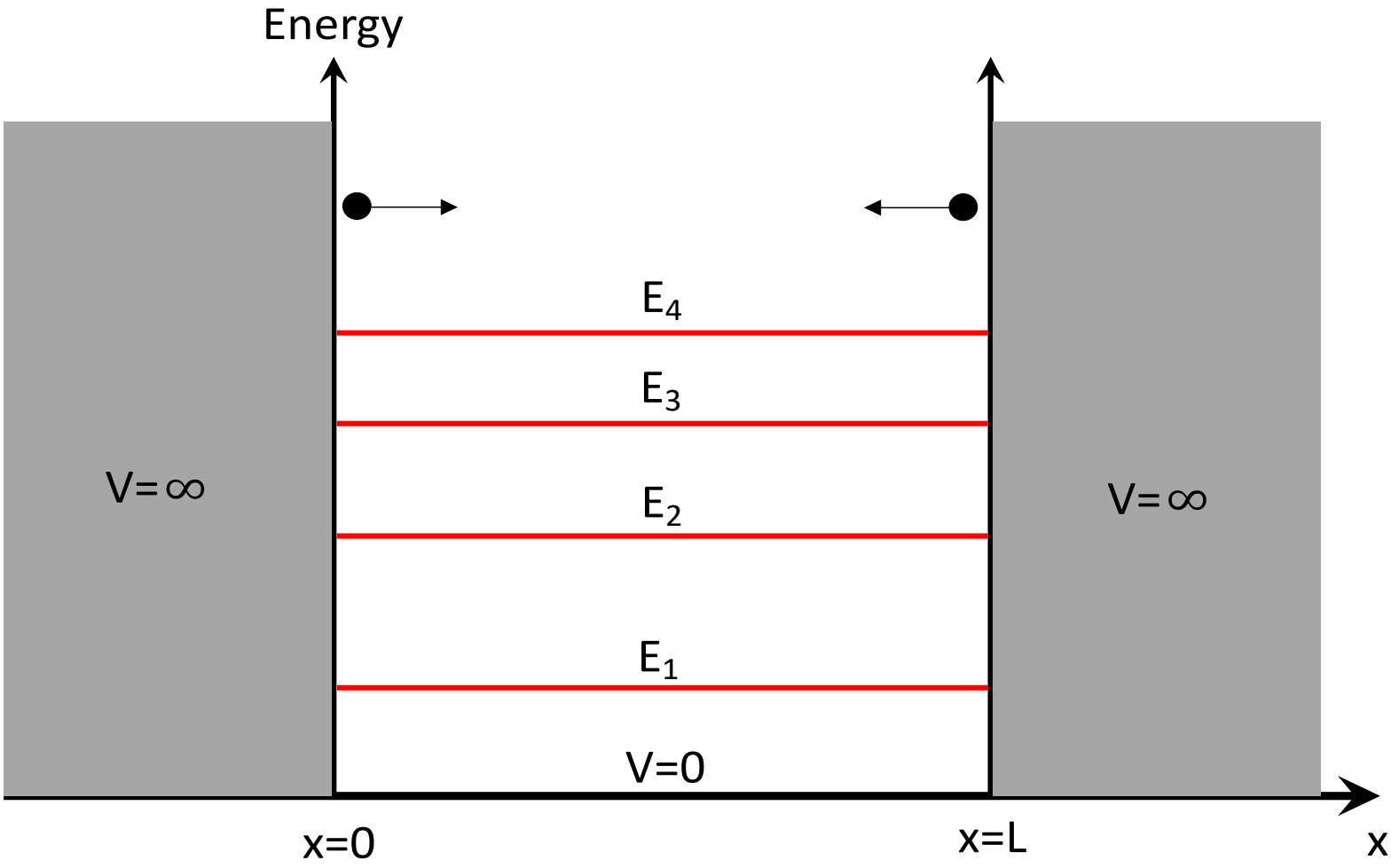
Imagine a particle is captured in a one-dimensional box. The particle moves back and forth, there's no other particles to interactive with, and there is no external motive.
The well is extended from $x = 0$ to $x = L$. The Schrödinger equation can be written as:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x) + V(x)\Psi(x) = E\Psi(x) \tag{8}$$

Questions

1. What is the physical meaning of the first term in the above equation?
2. How we can determine the boundary conditions for this specific problem?

Perfect 1D quantum well



Perfect 1D quantum well

In order to solve this type of PDEs (carrying physical dimensions) one makes them first dimensionless. To do so, we can define a characteristic value (available in the system) for a specific dimension.

For example, we define the length of the well as a characteristic length L and normalize the x coordinate by this value:

$$x \in [0, L] \rightarrow \text{define } x' = x/L \rightarrow x' \in [0, 1] \tag{9}$$

If we had a situation where

$$x \in [0, 2L] \rightarrow x' \in [0, 2] \tag{10}$$

Questions

- What about other dimensions in the Shrödinger equation?
- How do the Shrödinger equation and boundary condition look like?

Eigenvalues and Eigenfunctions

Analytics

- Using the dimensionless ODE and boundary conditions, we derive analytical expressions for the eignfunctions and eigenvalues of this moving particle. The eigenvalues are the allowed energies that a moving particle can occupy in this system.

We can start with an Ansatz

$$\Psi(x) = Ae^{ik_x x} + Be^{-ik_x x}, \tag{11}$$

and apply the boundary conditions and find proper values for A and B.

Eigenvalues and Eigenfunctions

Numerics

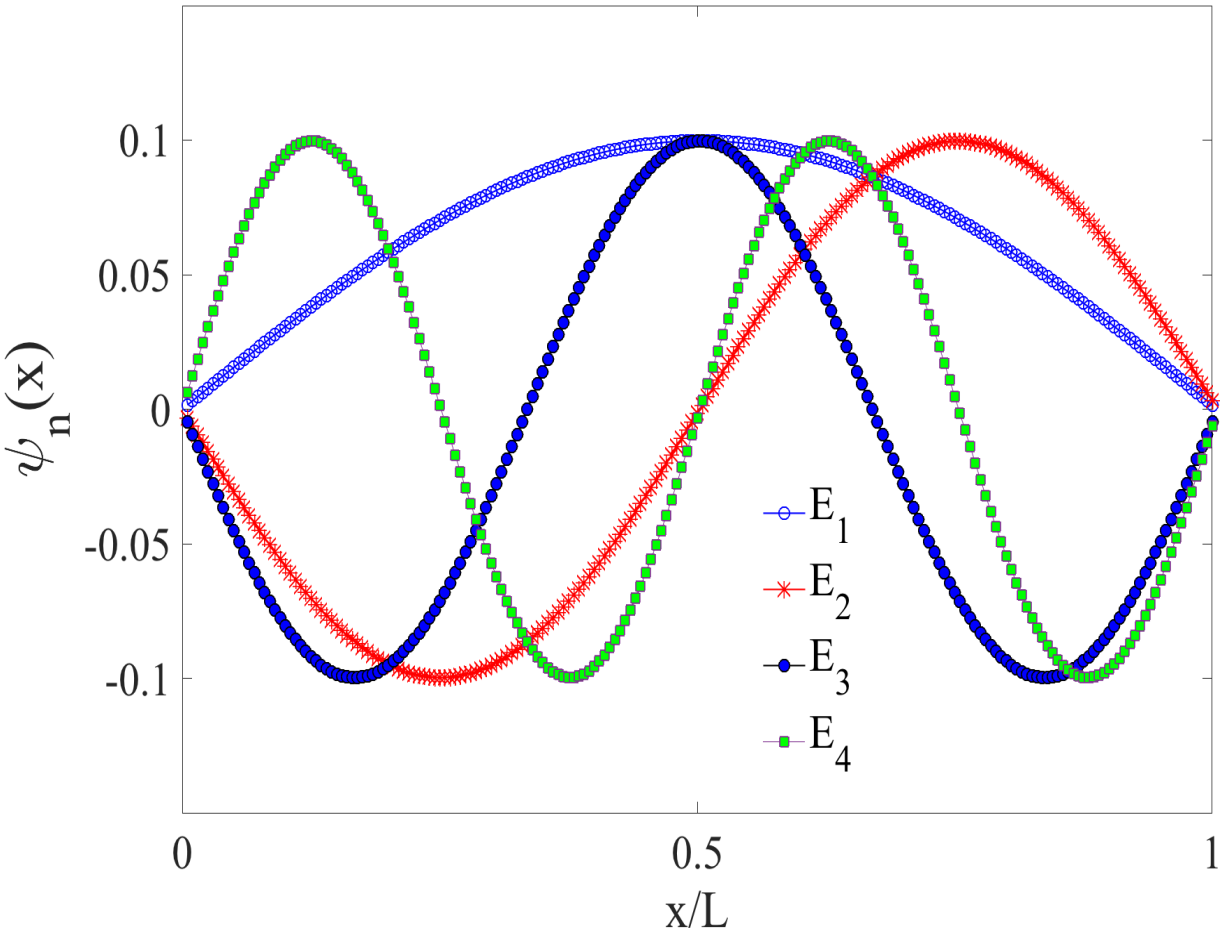
- Using a finite difference method (FDM), we solve the ODE with different step sizes for the discretization, say $\Delta x' = 0.1$ (equal to N=10 grid points).
  Remember that in a FDM, we write the first derivative by

$$\frac{\partial}{\partial_x}\Psi(x) \approx \frac{1}{\Delta x}[\Psi(x+\Delta x) - \Psi(x)]\Big|_{\Delta x \to 0} \tag{12}$$

- In order to compare our numerical results with analytics, we plot the first eigenfunction we find using FDM and the exact solution in a single frame. We repeat it for few more cases.
- We also do the same for the eigenvalues.

Eigenvalues and Eigenfunctions

An example of calculated wavefunctions:



Eigenvalues and Eigenfunctions

- To figure out the relation between N, the number of grid points, and error introduced, we define two error functions: One for the eigenvalues and one for the eigenvectors (not for all of them. Only a first few) and plot them as a function of N or $\Delta x'$.
  We expect that by increasing N or equivalently decreasing $\Delta x'$ the error functions decay.

Eigenvalues and Eigenfunctions

A generic vector $\mathbf{V}$ in a coordinate system is defined by the unit vectors of this specific coordinate system.

$$\mathbf{V} = V_x \mathbf{e}_x + V_y \mathbf{e}_y + V_z \mathbf{e}_z \tag{13}$$

The unit vectors are orthogonal, namely, their inner product is zero, i.e.

$$\begin{cases} \mathbf{e}_i \cdot \mathbf{e}_j = 0, \\ \mathbf{e}_i \cdot \mathbf{e}_i = 1. \end{cases} \tag{14}$$

In other words, they do not have any projection on each other.

In quantum mechanics one can also find closed sets of bases and describe any generic wavefunction Ψ_0 by them. Let's assume $\{\Psi_n\}$ is a closed set. The following relation returns the projections of Ψ_0 on $\{\Psi_n\}$:

$$\alpha_n = \int \int dt d\mathbf{r}\, \Psi_n^*(\mathbf{r}, t) \Psi_0(\mathbf{r}, t) \tag{15}$$

Once $\alpha_n = 0$, the wavevector Ψ_0 has no projection on component Ψ_n.

Time propagation using H(**r**)

We can check it for our own case. To do so, we use the following integral

$$\alpha_{nm} = \int dx\, \Psi_n^*(x)\Psi_m(x) \tag{16}$$

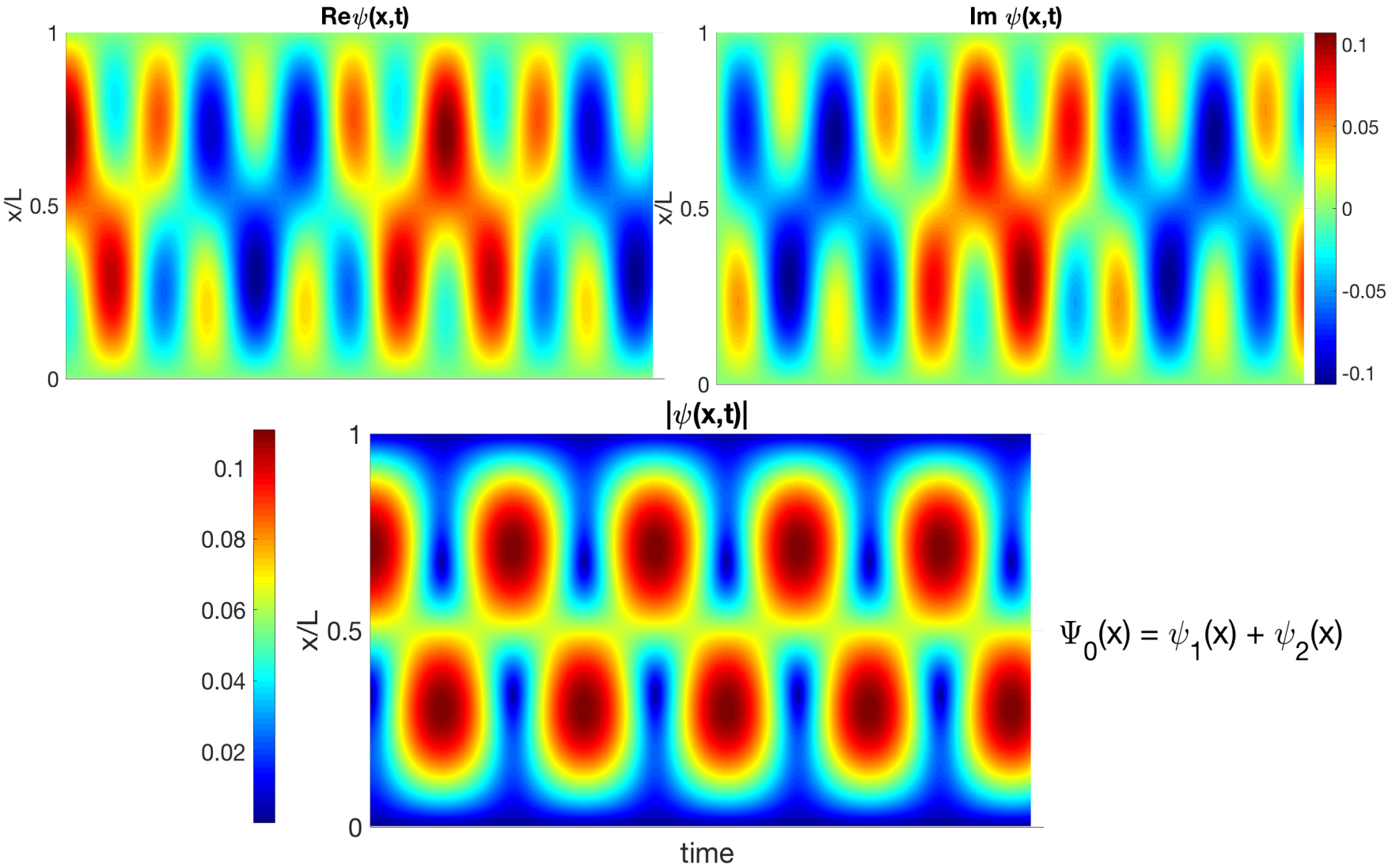
where Ψ_n (or Ψ_m) is the nth (or mth) eigenfunction we obtain using our numerics. We should try cases where $n = m$ and $n \neq m$.
What do the results mean?

Once we have α_n we can study the propagation of an initial state Ψ_0 in time:

$$\Psi(x,t) = \sum_n \alpha_n e^{-iEt/\hbar}\psi_n(x) \tag{17}$$

- We should investigate the evolution of two initial eigenvectors using our numerically computed eigenstates:
  (1) $\Psi_0(x') = \psi_1(x')$
  (2) $\Psi_0(x') = \delta(x' - 1/2)$

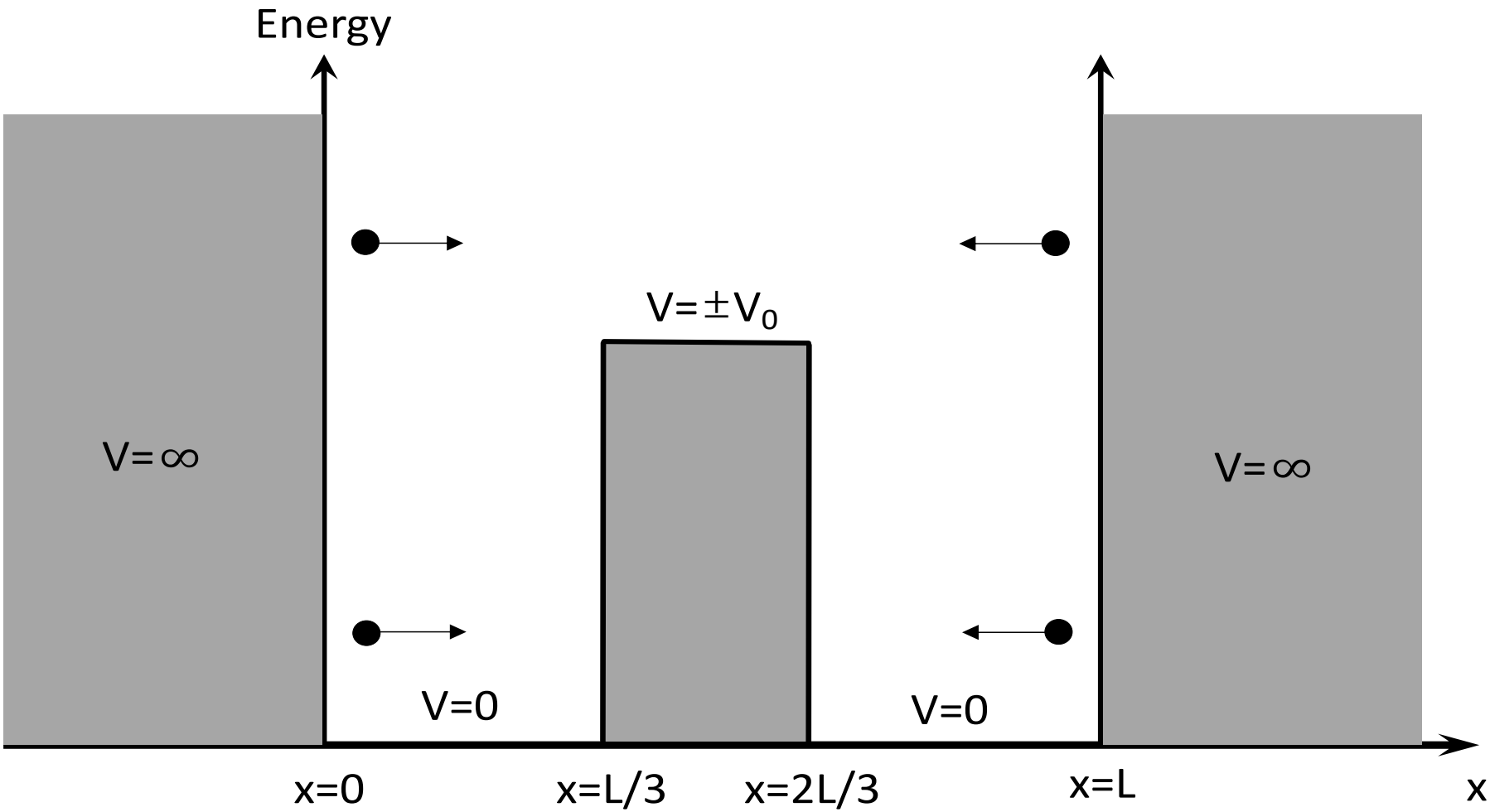
Time propagation using H(**r**)



$$\Psi_0(x) = \psi_1(x) + \psi_2(x)$$

Perturbed 1D quantum well

Now consider a situation where the quantum well is distorted by a potential barrier V_0 at the middle.



Perturbed 1D quantum well

- Similar to the previous case, we should find the eigenstates and eigenvalues
- Also we investigate the propagation of an initial state using the eigenfunctions we obtain

How many states are located below $V = +V_0$?
This number should be equal to the number of roots of the following expression.

$$f(\lambda) = \mathrm{e}^{\frac{\kappa}{3}} \left[\kappa \sin\left(\frac{k}{3}\right) + k \cos\left(\frac{k}{3}\right)\right]^2 - \mathrm{e}^{-\frac{\kappa}{3}} \left[\kappa \sin\left(\frac{k}{3}\right) - k \cos\left(\frac{k}{3}\right)\right]^2, \tag{18}$$

$k = \sqrt{\lambda}$ and $\kappa = \sqrt{\nu_0 - \lambda}$

Time propagation using H(**r**,t)

When the Hamiltonian is explicitly time-dependent we are unable to use the previous scheme to study the propagation of states in time.

$$\Psi(x,t') = e^{-iH(t')\Delta t}\Psi(x,t), \quad t' = t + \Delta t, \;\; \Delta t \to 0 \tag{19}$$

Tylor expanssion:

$$\Psi(x,t') = e^{-iH(t')\Delta t}\Psi(x,t) = \Big[1 - iH(t')\Delta t\Big]\Psi(x,t) \tag{20}$$

Forward Euler approximation
Not Hermitian and thus does not preserve the norm of wavefunction.

Time propagation using H(**r**,t)

In order to find a Hermitian time-propagator, we make use of the Crank-Nicolson scheme

$$\Psi(x,t') = e^{-iH(t')\Delta t/2} e^{-iH(t')\Delta t/2} \Psi(x,t) \tag{21}$$

$$e^{+iH(t')\frac{\Delta t}{2}} \Psi(x,t') = e^{-iH(t')\frac{\Delta t}{2}} \Psi(x,t) \tag{22}$$

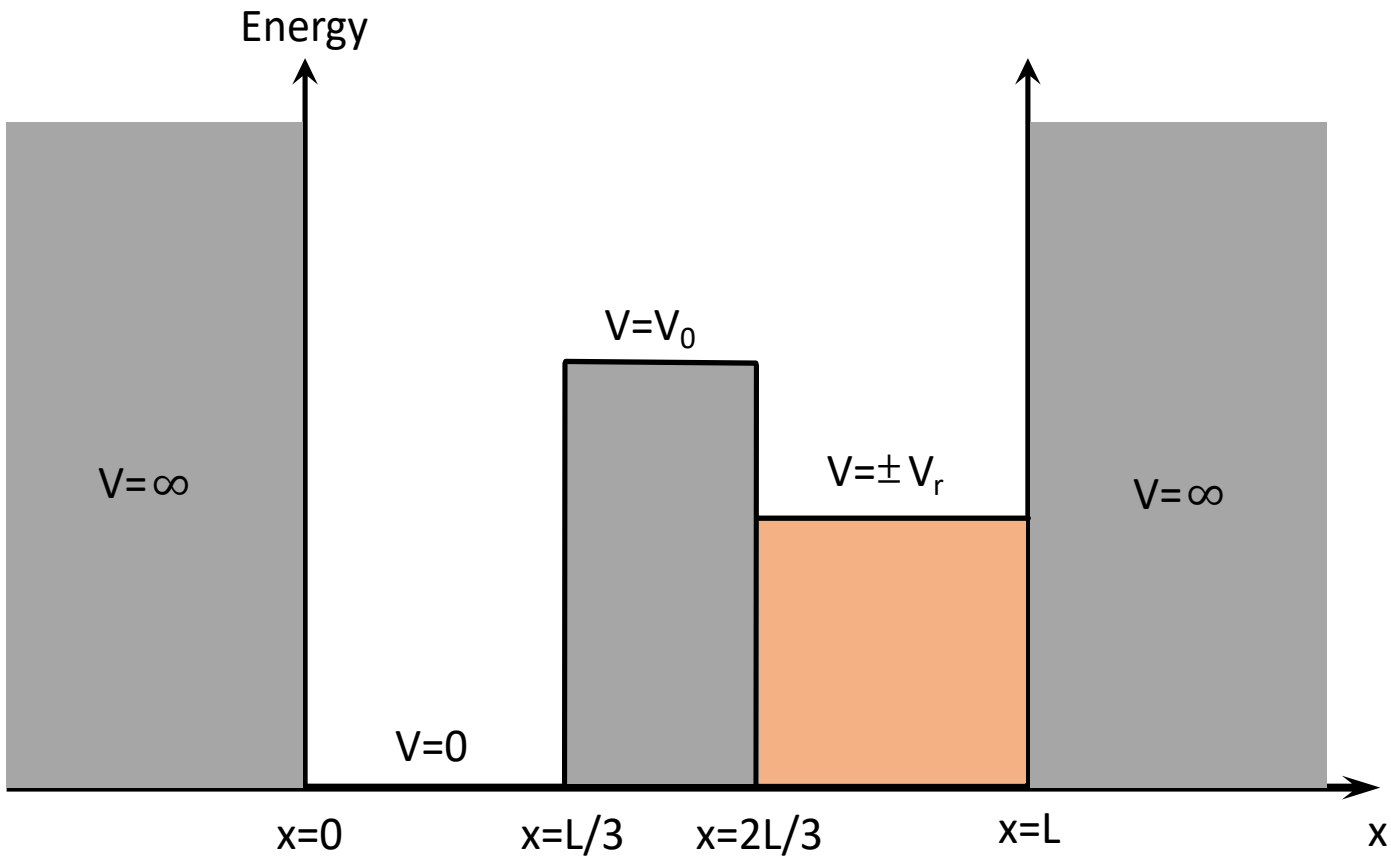
$$\left[1 + iH(t')\frac{\Delta t}{2}\right] \Psi(x,t') = \left[1 - iH(t')\frac{\Delta t}{2}\right] \Psi(x,t) \tag{23}$$

$$U(x,t') = \frac{1 - iH(x,t')\frac{\Delta t}{2}}{1 + iH(x,t')\frac{\Delta t}{2}}, \quad \Psi(x,t') = U(x,t')\Psi(x,t) \tag{24}$$

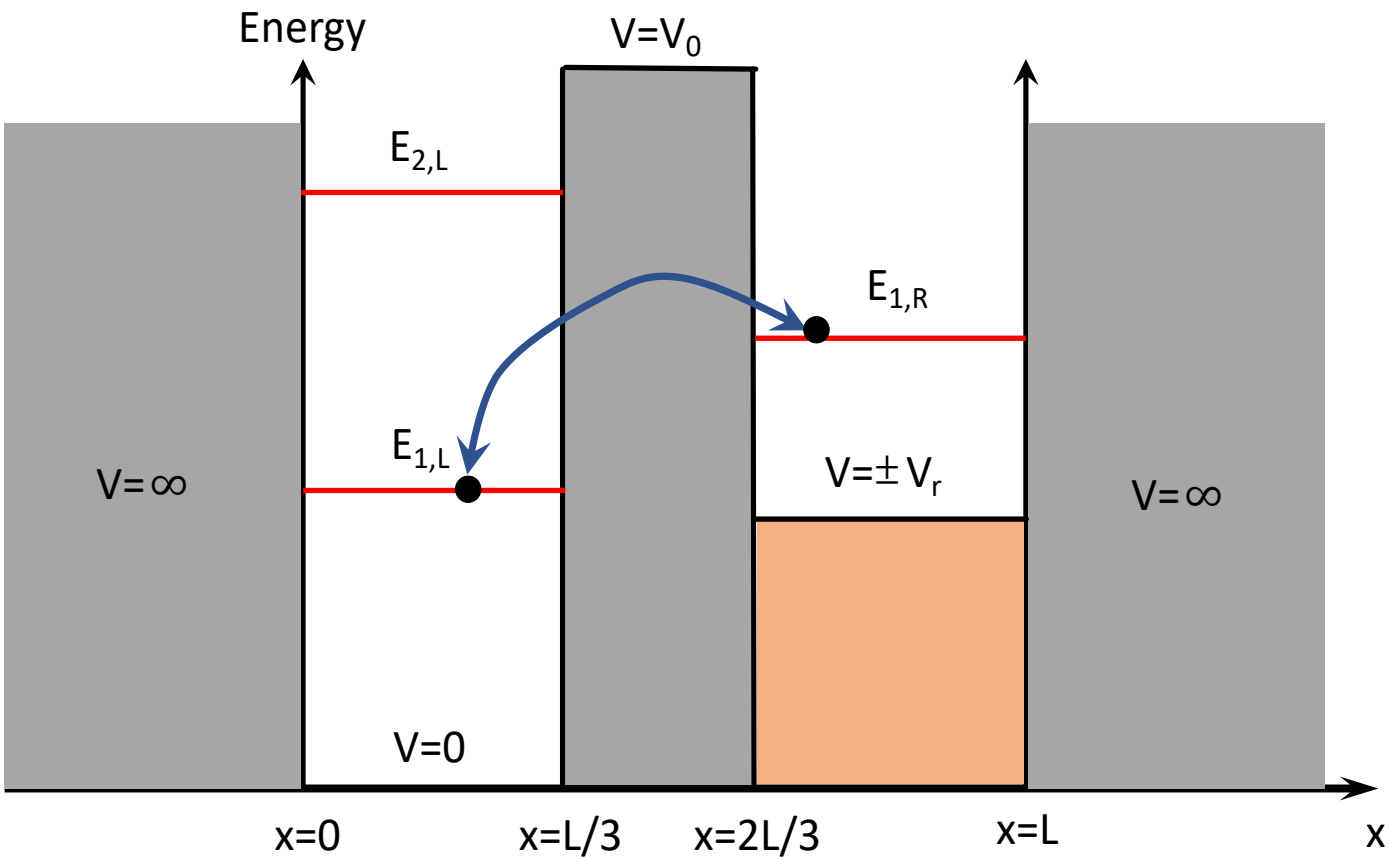
- Check if $U(x,t')$ is unitary?
- Compare your results of previous tasks with those you get by this method.

Time-dependent 1D coupled quantum wells

Consider a situation where the potential at the right side of the barrier oscillates. It can be a barrier-like or finite-well-like. This fictitious problem allows to study time-dependent population transfer from one quantum state to another without applying an explicit time-dependent approach.



Time-dependent 1D coupled quantum wells



Time-dependent two-level system

We can define an effective Hamiltonian out of these two level like this

$$H_{eff} = \begin{pmatrix} E_{1,L} & \tau_{1L,1R}(V) \\ \tau_{1R,1L}(V) & E_{1,R} \end{pmatrix} \tag{25}$$

$$\tau(V) = \int_0^L dx \psi^*_{1,L}(x) H(x,V) \psi_{1,R}(x) \tag{26}$$

- We should investigate the tunnel coupling between these two states.

Time-dependent two-level system

Imagine the previous two-level system where the coupling between the two states is an oscillatory function in time:

$$H_0 + V(t) = \begin{pmatrix} +E_0/2 & 0 \\ 0 & -E_0/2 \end{pmatrix} + \begin{pmatrix} 0 & \tau_0 \sin(\omega t) \\ \tau_0 \sin(\omega t) & 0 \end{pmatrix} \tag{27}$$

The formal solution to the Shrödinger equation at time t is given by:

$$\Psi(t) = \Psi(t_0) - \frac{i}{\hbar} \int_{t_0}^{t} dt' \left[H_0(t') + V(t') \right] \Psi(t') \tag{28}$$

where $\Psi(t_0)$ is the known initial wavefunction at time t_0.

Time-dependent two-level system

In the interaction picture this integral takes the form

$$\Psi(t) = \Psi(t_0) - \frac{i}{\hbar}\int_{t_0}^{t} dt' V_{\mathrm{I}}(t')\Psi(t'), \tag{29}$$

with $V_{\mathrm{I}}(t') = e^{iH_0 t'/\hbar} V(t') e^{-iH_0 t'/\hbar}$. This is a Volterra integral equation of the second kind and it has a simple analytical solution when $\omega = E_0$.

Time-dependent two-level system

To find a numerical solution we can use a collocation method:

- Discterize the integral using a method that you consider most convenient (Newton-Cotes quadrature, etc.)
- For each time $t = k\,\Delta t$ we obtain:

$$\hat{\mathbf{M}}(k\,\Delta t)\cdot\mathbf{f}(k\,\Delta t) = \mathbf{f}(t=0) + \sum_{r=0}^{k-1}\hat{\mathbf{N}}(r\,\Delta t)\cdot\mathbf{f}(r\,\Delta t), \qquad (30)$$

  with $\hat{\mathbf{M}}$ and $\hat{\mathbf{N}}$ two 2×2 matrices and $\mathbf{f}$ the two-component vector that we want to find.
- For each time $t = k\,\Delta t$ solve the emerging system of linear equations

Time-dependent two-level system

- Once we have $\Psi(t)$, obtain the probability of finding system in a state ψ_0

$$p(t) = |\langle \psi_0 | \Psi(t) \rangle| \tag{31}$$

- We should compare our results to an analytically obtained expression for this probability, namely:

$$p(t) = \sin^2\left(\frac{t\tau}{2\hbar}\right) \tag{32}$$