FY8904 Assignment 2

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Spring 2019

Abstract

We have studied the particle in a box and the double well problem, using computational physics, comparing the results to analytical/exact results where possible. We have found that using expansion in eigenstates reproduces analytical results well, and modelled quantum tunnelling in the double well system using this method. The tunnelling problem was also solved using a Crank-Nicholson finite difference scheme, which reproduced the earlier results well. We found the analytial tunnelling time to match the model results well. In the double well we found the ground states to be not degenerate, as expected.

Theory

The Schrödinger equation

The one-dimensional Schrödinger equations in dimensionless form reads (time-dependent)

$$i2mL^2\frac{\partial\Psi}{\partial t'} = \hat{H}\Psi \tag{1}$$

and (time-independent)

$$E_n\psi_n = \hat{H}\psi_n, \tag{2}$$

where E_n is the energy of the state ψ_n.

We have chosen the non-dimensionalizing scales

$$\frac{t}{t'} = t_0 = \frac{2mL^2}{\hbar} \quad \text{and} \quad \frac{x}{x'} = x_0 = L, \tag{3}$$

where L is the size of the domain (the width of the infinite well in our case).

Particle in a box

For the particle in a box problem the boundary conditions are

$$\Psi(x'=0,t') = 0 \quad \text{and} \quad \Psi(x'=1,t') = 0, \tag{4}$$

and the (dimensionless) Hamiltonian is

$$\hat{H} = -\frac{\partial^2}{\partial x'^2} + \nu(x'), \tag{5}$$

where $\nu(x' \in [0,1]) = 0$ and $\nu(x') = \infty$ elsewhere. The exact solution of Eq. (2) is

$$\psi_n(x') = \sqrt{2}\sin\left(n\pi x'\right) \quad \text{for} \quad n = 1,2,3,\ldots \tag{6}$$

with eigenvalues $\lambda_n = (\pi n)^2$. The relation between λ_n and E_n is

$$\lambda_n = E_n\frac{2mL^2}{\hbar^2}. \tag{7}$$

Box with potential barrier/double well

For a box with a potential barrier the potential is modified as follows

$$\nu(x') = \begin{cases} 0 & \text{for } 0 < x' < 1/3 \\ \nu_0 & \text{for } 1/3 < x' < 2/3 \\ 0 & \text{for } 2/3 < x' < 1 \\ \infty & \text{otherwise,} \end{cases} \tag{8}$$

where $\nu_0 = t_0V_0/\hbar$ is a dimensionless measure of the strength of the potential barrier.

Periodic detuning of a two-level system

Introducing a time-dependent potential

$$\nu(x') = \begin{cases} 0 & \text{for } 0 < x' < 1/3 \\ \nu_0 & \text{for } 1/3 < x' < 2/3 \\ \nu_r(t) & \text{for } 2/3 < x' < 1 \\ \infty & \text{otherwise,} \end{cases} \tag{9}$$

we can force population transfers between the two lowest energy levels.

Expansion in eigenfunctions

If we know the expansion of the initial condition Ψ_0 in the eigenfunctions ψ_n

$$\Psi_0(x') = \sum_n \alpha_n\psi_n(x') \tag{10}$$

then the Schrödinger equation gives us the time evolution of the system

$$\Psi(x',t') = \sum_n \alpha_n \exp\left(-i\lambda_n t'\right)\psi_n(x'). \tag{11}$$

The coefficients α_n can be calculated using the inner product between the initial state Ψ_0 and the eigenstates ψ_n

$$\alpha_n = \langle\psi_n, \Psi_0\rangle = \int \psi_n^*(x')\Psi_0(x')\,\mathrm{d}x'. \tag{12}$$

Finite difference time evolution

If we have a time-dependent Hamiltonian the method of expansion in eigenfunctions can not be used. An alternative method for time evolution is finite difference methods. We then use the formal solution of the Schrödinger equation for two times separated by $\Delta t'$

$$\Psi(x',t'+\Delta t') = \exp(-i\Delta t'\hat{H})\Psi(x',t'). \tag{13}$$

One approximation to this equation is the forward Euler scheme

$$\Psi(x', t' + \Delta t') = \left[1 - i\Delta t' \hat{H}\right] \Psi(x', t'). \tag{14}$$

This scheme does not preserve probabilities, since the approximation to the time evolution operator $\exp(-i\Delta t' \hat{H})$ is not unitary. A better choice is the Crank-Nicholson scheme

$$\left[1 + \frac{i}{2}\Delta t' \hat{H}\right] \Psi(x', t'+\Delta t') = \left[1 - \frac{i}{2}\Delta t' \hat{H}\right] \Psi(x', t'+\Delta t'). \tag{15}$$

Numerical details

We solve the Schrödinger equations using finite difference, using the forward difference for the first derivative

$$\frac{\partial f(x)}{\partial x} \approx \frac{f(x + \Delta x) - f(x)}{\Delta x} \tag{16}$$

and the central difference for the second derivative

$$\frac{\partial^2 f(x)}{\partial x^2} \approx \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2}. \tag{17}$$

This allows us to rewrite the Schrödinger equations as an eigenvalue problem $(\boldsymbol{A} - \lambda_n \boldsymbol{I})\boldsymbol{x} = 0$ ($\boldsymbol{I}$ is the identity matrix), which is solved using the `numpy` function `numpy.linalg.eigh`.

When setting up the matrix $\boldsymbol{A}$ we don't include the boundaries $\Psi(x = 0)$ and $\Psi(x = L)$, since these are known to always be equal to zero, due to the infinite potential. This gives wave functions that are exactly equation to the analytical solution (within machine precision), no matter which Δx we choose, as can be seen for example in Fig. 1.

Results and discussion

Particle in a box

In Fig. 1 the numerically estimated eigenvalues (left) and eigenfunctions (right) are plotted together with the exact results from Eq. (6), for an infinite well with $\Delta x' = 1/200$. We see that the eigenfunction match the analytical solution perfectly, but that there is some discrepancy in the eigenvalues at n greater than approx. 30.

In Fig. 2 the time development of the particle in a box is plotted for the initial condition $\Psi_0 = \psi_1$, the first eigenfunction. We see that $|\Psi|^2$ is constant in time, but that Ψ itself oscillates between fully real and fully imaginary (and everything in between).

Using a delta function as initial condition $\Psi_0(x) = \delta(x - 1/2)$ fixes the initial position of the particle at $x = 1/2$. This results in coefficients

$$\alpha_n = \int \psi_n^*(x)\delta(x - 1/2)\,\mathrm{d}x = \psi_n^*(x = 1/2), \tag{18}$$

which means that the initial wave function will be a combination of all eigenfunctions ψ_n. To properly represent this we need to include an infinite number of eigenfunctions. Further, since we have an exact position (with *infinite certainty*) means that we have *infinite uncertainty* in

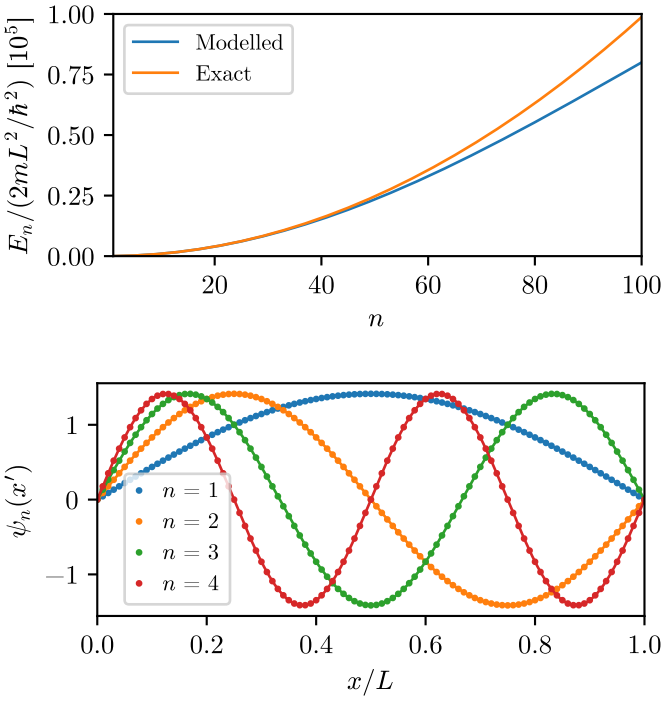

Figure 1: Eigenvalues (top) and eigenfunctions (bottom) in an infinite well with $\Delta x' = 1/200$. The exact eigenvalues $\lambda_n = (\pi n)^2$ and eigenfunctions Eq. (6) are also shown.

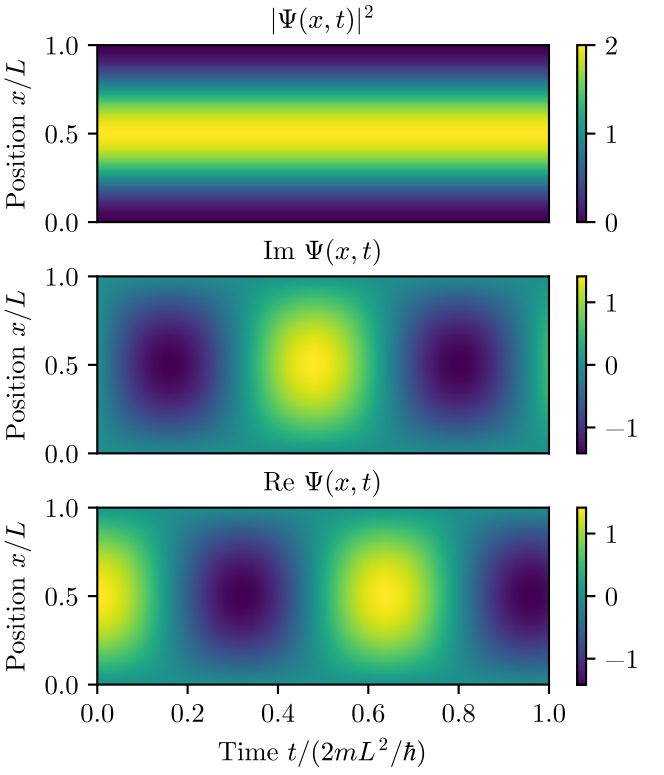

Figure 2: Time-development of particle in a well with initial condition $\Psi_0(x', t' = 0) = \psi_1$ and $\Delta x' = 1/200$ and $\Delta t' = 1/2000$.

the momentum of the particle, following the uncertainty princinple. This means that any results for $t > 0$ will not make any sense. Now, the numerical simulations doesn't know that this is not possible, so it willingly spits out results like the ones in Fig. 3. The simulations can not use an infinite number of eigenfunctions to represent the initial condition, so in practice we are probably seeing the results of using a bad approximation of a triangle wave or a Gaussian as initial condition.

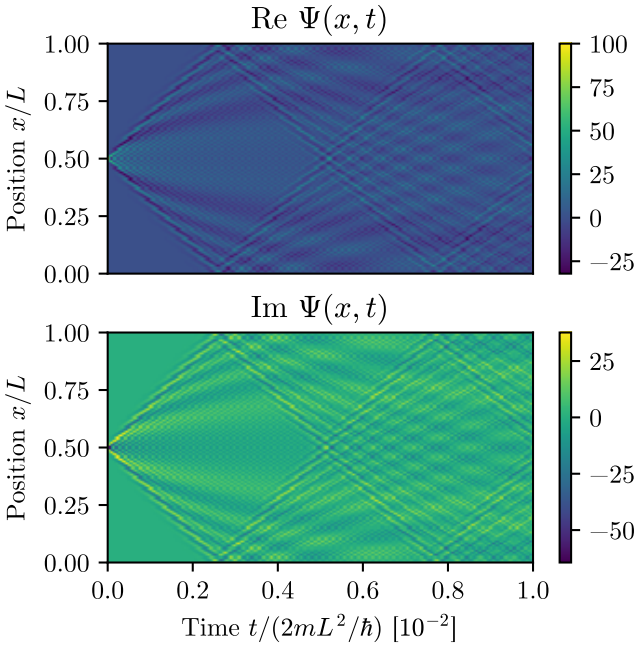

Figure 3: Time-development of particle in a well with initial condition $\Psi_0(x', t' = 0) = \delta(x' - 1/2)$ and $\Delta x' = 1/200$ and $\Delta t' = 10^{-5}$.

Double well

In Fig. 5 we have plots of the first three eigenfunctions of the double well (right), and the first eigenvalues. We see that the first excited state ($n = 2$) has nearly the same wave function as the ground state, but with odd parity (the blue line for $n = 1$ is hidden under the orange line for $n = 2$ in the left half of the plot).

The first 6 eigenvalues are given below. We see that the first excited state (λ_2) is *nearly* degenerate with the ground state (λ_1), and similarly for λ_3 and λ_4, and λ_5 and λ_6. The states are not fully degenerate because we cannot have degeneracy in a 1D system like this.

$$\lambda_1 = 73.8663877 \quad \lambda_2 = 293.2169877 \quad \lambda_4 = 647.6674955$$
$$\lambda_2 = 73.8683378 \quad \lambda_3 = 293.2410202 \quad \lambda_5 = 648.1536705$$

In Fig. 5 plots of the probability density is given. We see that the probability density is concentrated the left side of the barrier at $t' = 0$, and that it tunnels through the barrier and is fully concentrated on the right side of the barrier at $T = t' = \pi/(\lambda_2 - \lambda_1)$. The tunnelling time T is the (half) period of the exponential of Eq. (11).

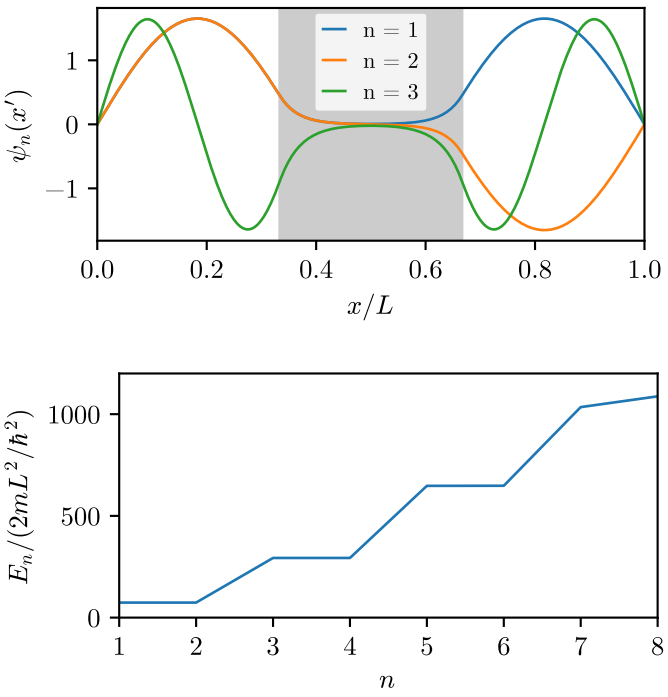

Figure 4: Eigenfunctions (top) and eigenvalues (bottom) in a double well with $\Delta x' = 1/1000$ and $\nu_0 = 1000$. The middle barrier is indicated by the central gray area.

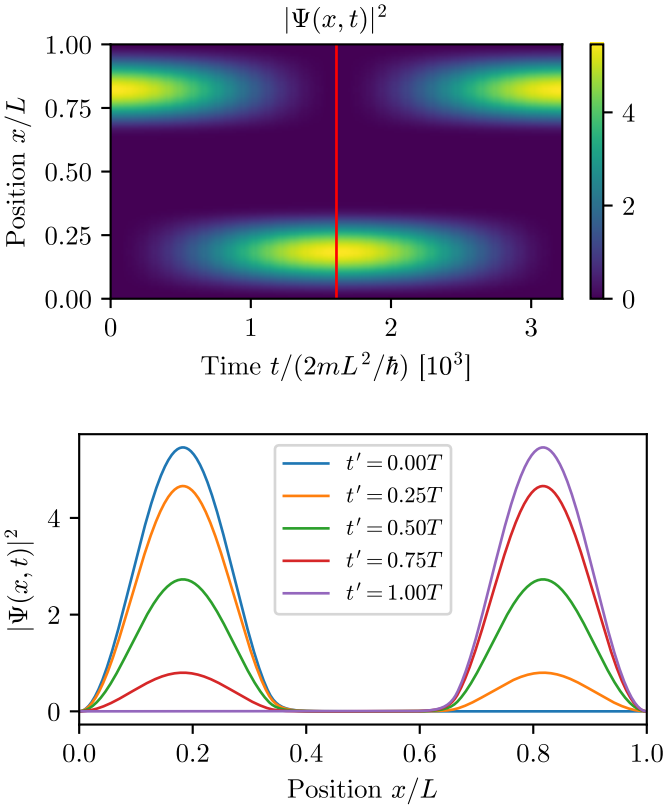

Figure 5: Time evolution of the double well with initial condition $\Psi_0 = 1/\sqrt{(2)}(\psi_1 + \psi_2)$, $\Delta x' = 1/1000$ and $\nu_0 = 1000$. T is the tunnelling time $t' = \pi/(\lambda_2 - \lambda_1)$, and is indicated by the red vertical line in the top figure.

Root-finding

It can be shown that the eigenvectors of the Hamiltonian with energies $0 < \lambda < \nu_0$ are given by the equation

$$f(\lambda) = e^{\kappa/3}\left[\kappa \sin\left(\frac{k}{3}\right) + k\cos\left(\frac{k}{3}\right)\right]^2 - e^{-\kappa/3}\left[\kappa \sin\left(\frac{k}{3}\right) - k\cos\left(\frac{k}{3}\right)\right]^2 = 0, \quad (19)$$

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

We find the roots of Eq. (19) using the function `scipy.optimize.root` from the `Python`-package `SciPy`, with the default `hybr` method. This uses a modification of the Powell's hybrid method[1] implemented in MINPACK's `hybrd` and `hybrj` routines. Other methods can be selected using the `method` argument, but we found the default method to give sufficient results. We use the eigenvalues λ_1 to λ_6 from before as starting points for the function.

The resulting roots are listed below, and a plot of Eq. (19) with the roots indicated by vertical lines is shown in Fig. 6. We see that the roots of Eq. (19) doesn't perfectly agree with the eigenvalues found before.

$\lambda_1 = 73.937533$ $\lambda_3 = 293.516198$ $\lambda_5 = 648.750278$
$\lambda_2 = 73.935600$ $\lambda_4 = 293.492315$ $\lambda_6 = 648.264373$

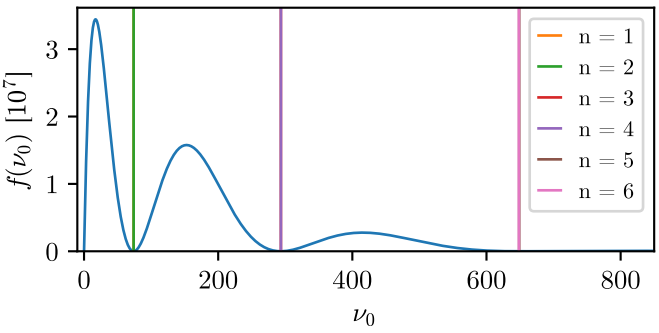

Figure 6: Plot of Eq. (19), with the roots indicated by vertical lines. The lines for $n = 1$ and $n = 2$ overlap, as does $n = 3$ and $n = 4$ etc.

In Fig. 7 we have plots of the number of eigenstates with eigenvalues lower than the barrier height ν_0. We find that the barrier height that separates having none and one such eigenstate is approximately $\nu_0 = 22.2$.

Finite difference time evolution

In Fig. 8 is a plot of $\int |\Psi(x,t)|^2 \, \mathrm{d}x'$ as a function of time for different simulations using the Euler scheme Eq. (14). We see that the solution diverges after some time, independent of the CLF-number.

In Fig. 9 we have plotted the time evolution of the double well using the Crank-Nicholson scheme Eq. (15). We have reduced the barrier height to $\nu_0 = 500$ to lower the tunnelling time, since the CN method requires $\Delta t' = \Delta x'^2$, so

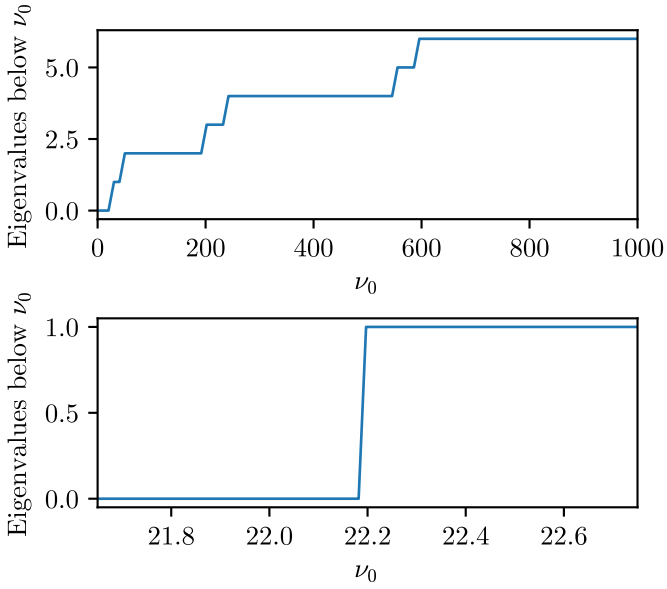

Figure 7: Plots of the number of eigenstates with eigenvalues less than the barrier height ν_0, as function of ν_0.

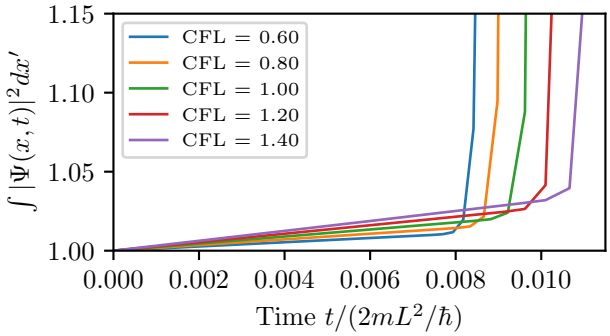

Figure 8: Plot of $\int |\Psi(x,t)|^2 \, \mathrm{d}x'$ as a function of time using the Euler scheme Eq. (14), for different CFL-numbers. We used $\Delta x' = 1/50$ and $\Delta t' = \Delta x'^2$ and initial state $\Psi = \psi_1$.

it would require too many time steps to do with the previous barrier height. We see that this method does not give divering proabilities, and that the tunnelling is observed at $t = \pi/(\lambda_2 - \lambda_1)$ as expected.

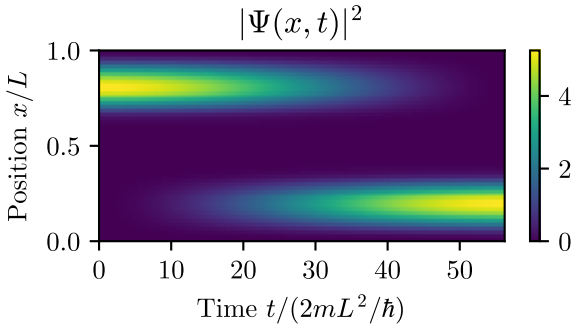

Figure 9: Time evolution of the double well with initial condition $\Psi_0 = 1/\sqrt{2}(\psi_1 + \psi_2)$, $\Delta x' = 1/50$ and $\nu_0 = 500$, using the Crank-Nicholson scheme.

The CN method is more computationally expensive than

the expansion in eigenstates, but if we for example have a time-dependent Hamiltonian it's not possible to use expansion in eigenstates.

Two-level double well system

In the left plot in Fig. 10 there is a plot of the two lowest eigenvalues λ_1 and λ_2 as function of the potential ν_r. In the right plot the two lowest eigenfunctions are plotted for positive and negative ν_r. We see that the ground state ψ_1 is localized at the left side for positive ν_r, and mostly located at the right side for negative ν_r, and vice versa for the excited state ψ_2.

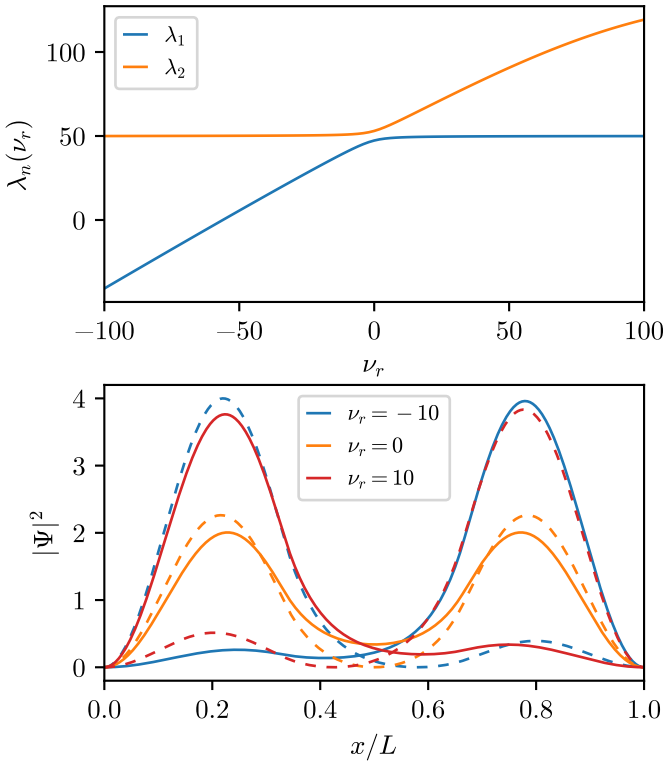

Figure 10: (top) Plot of the two lowest eigenvalues as function of ν_r with $\Delta x' = 1/1000$, and (bottom) localization of ground state with positive and negative ν_r. The solid lines show ψ_1 and dashed lines ψ_2.

Conclusion

We have modelled a particle in an infinite box by solving the time-independent Schrödinger equation as a eigenvalue matrix problem, which reproduced the analytical wave functions and eigenvalues well.

Using expansion in eigenstates we found the time development of a particle in a box. When a barrier was introduced in the center of the box tunnelling was observed at the expected time when using the initial condition $\Psi_0 = 1/\sqrt{2}(\psi_1 + \psi_2)$.

Using an Euler scheme for solving the time-dependent Schrödinger equation resulted in diverging wave functions, as expected. The Crank-Nicholson scheme worked better, and reproduced the tunnelling from before.

By finding the roots of an analytical expression for the eigenvectors of the Hamiltonian with energies less than the barrier height, we found the barrier height that separates having no such eigenstates and one such eigenstate was around $\nu_0 = 22.2$.

With a two-level double well system we found the ground state to be localized mostly at the left side for positive ν_r (the potential in the right hand well), and mostly at the right side for negative ν_r.

References

[1] M. J. Powell. "A hybrid method for nonlinear equations". In: *Numerical methods for nonlinear algebraic equations* (1970).

[2] S. L. Wakelin, J. T. Holt, and R. Proctor. "The influence of initial conditions and open boundary conditions on shelf circulation in a 3D ocean-shelf model of the North East Atlantic". In: *Ocean Dynamics* 59.1 (2009), pp. 67–81.