
Numerical analysis of position-dependent effective mass Schrödinger equation

(NUMERISK ANALYSE AF POSITION-AFHÆNGIG EFFEKTIVE MASSE
SCHRÖDINGER LIGNING)

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BACHELOR'S THESIS
SUBMITTED BY

KÅRE KOCH RØNNOW

STUD. NO.: 20112395

*Department of Physics and Astronomy,
Aarhus University*

SUPERVISED BY

DMITRI VLADIMIR FEDOROV

Abstract

English version

In this thesis the position-dependent effective mass Hamiltonian operator is sought for by making a 2-dimensional simulation and picking four Hamiltonian operators which are compared to simulation.

The method used for this is building the 2-dimensional simulation with a potential, which results in a movement along a curve, the increased length along the curve is equal to an increased effective mass. The four Hamiltonian operators are each put in their own 1-dimensional box and after changing coordinates their probability distributions become comparable.

The result of the thesis is that none of the four Hamiltonian operators is comparable in all three of the first states. For the ground state the Hamiltonian operator corresponding best was the first. For the first excited state the Hamiltonian operators corresponding best were the third and fourth, since they were so close together that it was not possible to tell which was the better. For the second excited state the Hamiltonian operator corresponding best was the second in the first and last third, while the first Hamiltonian operator corresponded best to simulation in the middle.

Dansk version

I dette projekt er den positions-afhængige effektive masse Hamilton operator søgt ved at lave en 2-dimensional simulering og vælge fire Hamilton operatorer at sammenligne med simuleringen.

Den anvendte metode til dette er at opbygge den 2-dimensional simulation således, at der er et potentiale, som resulterer i bevægelse langs en kurve. Længdeforøgelsen svarer til en forøgelse af den effektive masse. De fire Hamilton operator sættes i hver sin egen 1-dimensional kasse og efter et skift af koordinater sammenlignes sandsynlighedsfordelingerne.

Resultatet af projektet er, at ingen af de fire Hamilton operatorer svarer til simuleringen i de tre første tilstande. For grundtilstanden svarer den første Hamilton operator bedst. For den første exciterede tilstand svarer den tredje og fjerde Hamilton operator bedst, men så tæt på hinanden, at det ikke var muligt at se, hvilken der var bedst. For den anden exciterede tilstand svarer den anden bedst i første og sidste tredjedel, mens den første Hamilton operator svarer bedst i midten.

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Chapter 1

Introduction

The Schrödinger equation is one of the most useful and powerful equations in quantum mechanics, which is why it is such a limitation when it no longer applies because of its changing effective mass.

In a ever more digitalized world where computers and therefore semiconductors becomes more and more important a formula which can describe the motion of holes and electrons through semiconductors of different chemical compositions is of tremendous value.[1, p. 1]

To me, however, the usefulness of the increased knowledge of semiconductors is of lesser importance than the greater understanding of quantum mechanics and nuclear physics.

This thesis will look at four Hamiltonian operators and see if any of them could be the position-dependent effective mass Hamiltonian. This is done by making a 2-dimensional simulation of a position-dependent effective mass particle and thereafter taking the four different Hamiltonians in a 1-dimensional box. To make them comparable a change to similar coordinates is made and then the simulation, the Hamiltonian operators, and the analytical sine function probability distributions are all included into the same graphic. If one of the Hamiltonian operators is more consistent with the simulation it will be the position-dependent effective mass Hamiltonian. If none of them is more consistent to the simulation it will be tested which one is the closes to the simulation.

Chapter 2

The simulated system

The system is a plane where the particle moves along the x-axis with a built-in potential that forces the particle to move along the y-axis. How the particle moves in the y-axis is determined by a curve which is a function of x . The longer route the particle travels because of the potential corresponds to an increasing mass of the particle, and since the curve is dependent on position in x this increase in mass becomes position dependent, whereby becoming a simulation of a position-dependent effective mass particle.

2.1 Building the system

This simulation is a discrete Hamiltonian equation on a 2-dimensional quadrature grid, which is build using the method of Discrete Poisson equation on a two-dimensional rectangular grid [3], where instead of the equation $M_{correlation}\vec{u} = \vec{b}$ is solving $M_{correlation}\vec{u} = E\vec{u}$, $M_{correlation}$ being the correlation-matrix, \vec{u} a vector holding values for each point on the grid, and E an eigenvalue which corresponds to the energy.

The simulated system is build by making a plane of the area $L \times L$. On the plane the grid is made by placing point a on each corner and then dividing the sides between the corner points into equal lengths marked by points. Further points are placed in a quadrature grid based on the points on the sides.

Now that the grid is made, time has come to make correlations between points. For this the constant mass Hamiltonian operator is used[4, eq. 2.11]:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V \quad (2.1)$$

From this Hamiltonian operator a matrix with the correlation between each point on grid $M_{correlation}$ is made. All points along the sides must be 0, since the wave-function should not leave the 2-dimensional box. All other points have to be placed into vector \vec{u} , which starts with the point having the lowest x- and y-values continuing with the same x-value and all its y-values in increasing order. Then the next lowest x-value and all its increasing y-values etc. until all points are in this vector.

Taking the second derivative or finding the acceleration in 2 dimensions of the wave-function is done numerically using [3, First equation] where Δ is length between two points

$$\nabla^2 u_{ij} = \frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}}{\Delta^2}, \quad (2.2)$$

which can be done for all but the side-point, because the side-points are always 0 and therefore have the second derivative 0. However the side-points can still be used to calculate the second derivative, although they are not in the correlation-matrix, since they all have the value of 0.

To make sure that the wave-function follows the curve of the simulation there is added a potential to the simulation given by

$$V(x, y) = k(y - f(x))^2 \quad (2.3)$$

where the constant k has to be chosen large enough to force the wave-function follow the curve as tightly as is necessary for the simulation. The curves function $f(x)$ has to be chosen so that the starting and finishing values of V are the same. For this reason the Gaussian-function is chosen given by

$$f(x) = A + Be^{-(x-L/2)^2/a^2}, \quad (2.4)$$

A being the starting height, B the height of the curve, L is the length of the sides of the 2-dimensional box, and a determines the width of the curve. The potential only act on the point itself, therefore it will have to be added along the diagonal of the correlation-matrix.

A simple example of the correlation matrix, here for a 5×5 grid, is:

$$\begin{pmatrix} -4\frac{k^2}{2m\Delta^2} + V(x, y) & \frac{k^2}{2m\Delta^2} & 0 & \frac{k^2}{2m\Delta^2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{k^2}{2m\Delta^2} & -4\frac{k^2}{2m\Delta^2} + V(x, y) & \frac{k^2}{2m\Delta^2} & 0 & \frac{k^2}{2m\Delta^2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{k^2}{2m\Delta^2} & -4\frac{k^2}{2m\Delta^2} + V(x, y) & 0 & 0 & \frac{k^2}{2m\Delta^2} & 0 & 0 & 0 & 0 \\ \frac{k^2}{2m\Delta^2} & 0 & 0 & -4\frac{k^2}{2m\Delta^2} + V(x, y) & \frac{k^2}{2m\Delta^2} & 0 & \frac{k^2}{2m\Delta^2} & 0 & 0 & 0 \\ 0 & \frac{k^2}{2m\Delta^2} & 0 & \frac{k^2}{2m\Delta^2} & -4\frac{k^2}{2m\Delta^2} + V(x, y) & 0 & 0 & \frac{k^2}{2m\Delta^2} & 0 & 0 \\ 0 & 0 & \frac{k^2}{2m\Delta^2} & 0 & \frac{k^2}{2m\Delta^2} & -4\frac{k^2}{2m\Delta^2} + V(x, y) & 0 & 0 & \frac{k^2}{2m\Delta^2} & 0 \\ 0 & 0 & 0 & \frac{k^2}{2m\Delta^2} & 0 & 0 & -4\frac{k^2}{2m\Delta^2} + V(x, y) & \frac{k^2}{2m\Delta^2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{k^2}{2m\Delta^2} & 0 & \frac{k^2}{2m\Delta^2} & -4\frac{k^2}{2m\Delta^2} + V(x, y) & \frac{k^2}{2m\Delta^2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{k^2}{2m\Delta^2} & 0 & \frac{k^2}{2m\Delta^2} & -4\frac{k^2}{2m\Delta^2} + V(x, y) & \frac{k^2}{2m\Delta^2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{k^2}{2m\Delta^2} & 0 & -4\frac{k^2}{2m\Delta^2} + V(x, y) \end{pmatrix}$$

Now that the correlation-matrix is created the eigenvalues and eigenvectors can be found by using the routine `gsl_eigen_symmv` in GNU Scientific Library. The physical meaning of eigenvalue is the energy of the state. The physical meaning of eigenvectors is the wave-function, where each element of eigenvector is the wave-function in the corresponding element in \vec{u} . By sorting by the lowest eigenvalue in increasing order it is know which is the ground state, first excited state and so on.

Then by returning eigenvector elements to their corresponding points on the grid the wave-function of the state is found.

An example of wave-function of the ground state for the simulation can be seen at Figure 2.1.

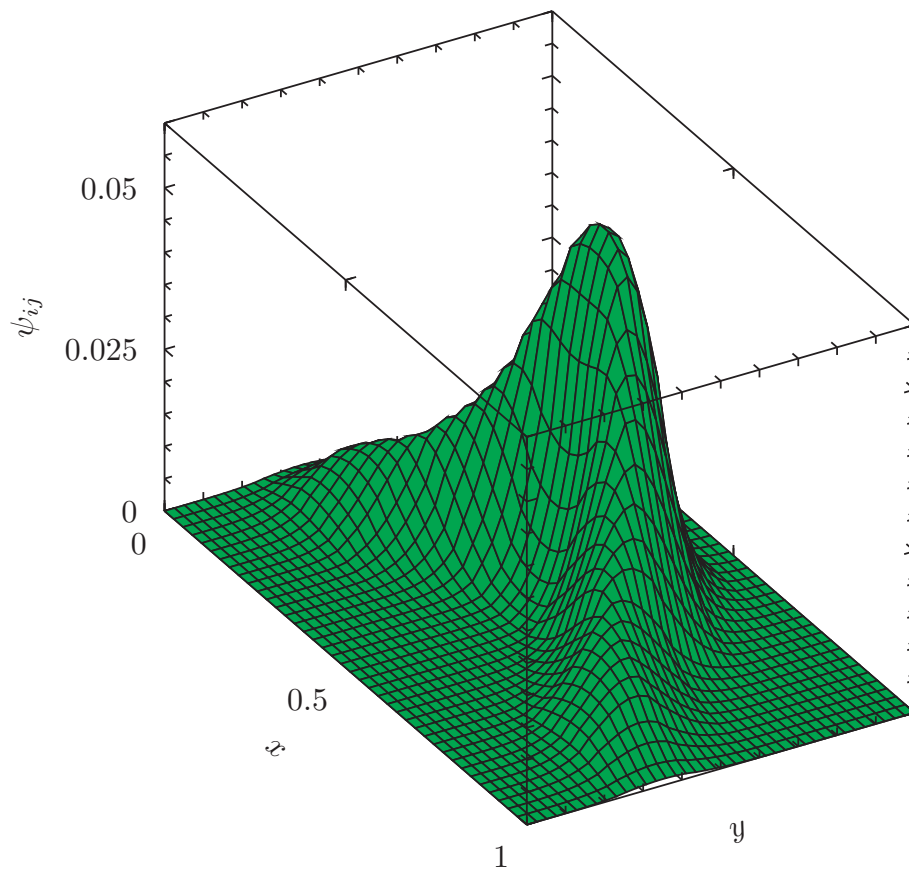


Figure 2.1: *The wave-function for the ground state of the simulation.*

Chapter 3

The 1 dimensional systems

Instead of having the position-dependence of the effective mass derived from a potential which result in movement along the y-axes, it will here be a 1-dimensional box along the s-axis, using the generalized Hamiltonian operator. The generalized Hamiltonian operator can generate a effective potential without the system having any potential. The hope is to find a Hamiltonian operator having the same effective potential as the built-in potential as the simulation.

3.1 Hamiltonian operators for the 1 dimensional systems

Since there is no potential in the systems the generalized Hamiltonian operator [1, eq. 6] simplifies to

$$\hat{H}_g = -\frac{\hbar^2}{4} \left(m(s)^\alpha \nabla m(s)^\beta \nabla m(s)^\gamma + m(s)^\gamma \nabla m(s)^\beta \nabla m(s)^\alpha \right). \quad (3.1)$$

The constants α , β and γ must satisfy the constraint [1, eq. 7]

$$\alpha + \beta + \gamma = -1 \quad (3.2)$$

In this thesis we compare the four different Hamiltonian operators to the position-dependent effective mass from the simulation.

The first Hamiltonian operator with the constants $\alpha = \gamma = 0$ and $\beta = -1$ becomes

$$\begin{aligned} \hat{H}_1 &= -\frac{\hbar^2}{2} \nabla \frac{1}{m(s)} \nabla \\ &= -\frac{\hbar^2}{2} \left(\frac{1}{m(s)} \nabla^2 - \frac{m'(s)}{m(s)^2} \nabla \right). \end{aligned} \quad (3.3)$$

The second Hamiltonian operator with the constants $\alpha = \gamma = -\frac{1}{4}$ and $\beta = -\frac{1}{2}$ becomes

$$\begin{aligned}
\hat{H}_2 &= -\frac{\hbar^2}{2} \frac{1}{\sqrt[4]{m(s)}} \nabla \frac{1}{\sqrt{m(s)}} \nabla \frac{1}{\sqrt[4]{m(s)}} \\
&= -\frac{\hbar^2}{2} \left(\frac{1}{m(s)} \nabla^2 - \frac{m'(s)}{m(s)^2} \nabla + \frac{7}{16} \frac{m'(s)^2}{m(s)^3} - \frac{1}{4} \frac{m''(s)}{m(s)^2} \right). \quad (3.4)
\end{aligned}$$

The third Hamiltonian operator with the constants $\alpha = -1$ and $\beta = \gamma = 0$ becomes

$$\begin{aligned}
\hat{H}_3 &= -\frac{\hbar^2}{4} \left(\frac{1}{m(s)} \nabla^2 + \nabla^2 \frac{1}{m(s)} \right) \\
&= -\frac{\hbar^2}{2} \left(\frac{1}{m(s)} \nabla^2 - \frac{m'(s)}{m(s)^2} \nabla + \frac{m'(s)^2}{m(s)^3} - \frac{1}{2} \frac{m''(s)}{m(s)^2} \right). \quad (3.5)
\end{aligned}$$

The fourth Hamiltonian operator with the constants $\alpha = \gamma = -\frac{1}{2}$ and $\beta = 0$ becomes

$$\begin{aligned}
\hat{H}_4 &= -\frac{\hbar^2}{2} \frac{1}{\sqrt{m(s)}} \nabla^2 \frac{1}{\sqrt{m(s)}} \\
&= -\frac{\hbar^2}{2} \left(\frac{1}{m(s)} \nabla^2 - \frac{m'(s)}{m(s)^2} \nabla + \frac{3}{4} \frac{m'(s)^2}{m(s)^3} - \frac{1}{2} \frac{m''(s)}{m(s)^2} \right). \quad (3.6)
\end{aligned}$$

3.2 Building the system

This simulation is a discrete Hamiltonian equation on a 1-dimensional line with equal intervals, which is build using a simplified version of the method of Discrete Poisson equation on a two-dimensional rectangular grid [3], where instead of the equation $M_{correlation} \vec{u} = \vec{b}$ is solving $M_{correlation} \vec{u} = E \vec{u}$. $M_{correlation}$ being the correlation-matrix, \vec{u} is a vector holding values for each point on the grid, and E is an eigenvalue corresponding to the energy.

The 1-dimensional Hamiltonian system is build by making a line of length L . On the line a point is set at the start and the end and divided by points with equal intervals.

Now that the intervals are made, correlations between points shall be made using the four derived Hamiltonian operators from section 3.1. The position-dependent effective mass $m(s)$ is given by

$$m(s) = m f(s), \quad (3.7)$$

m being the mass of the particle, and $f(s)$ the same function as in equation (2.4). Because the m is a constant it can be taken out of the brackets in the Hamiltonian operators.

For each of these Hamiltonian operators a matrix with the correlation between each point on line $M_{correlation}$ is made. The values of the start- and

the end-points the must be 0, since the wave-function should not leave the 1-dimensional box. All other points have to be placed into at vector \vec{u} , which starts from the point with the lowest s -value and continues for all s in increasing order.

Taking the second derivative or finding the acceleration in 1 dimension of the wave-function is done numerically using [5, eq. 5.6] where Δ is length between two points

$$\nabla^2 u_i = \frac{u_{i+1} + u_{i-1} - 2u_i}{\Delta^2}, \quad (3.8)$$

which can be done for all but the first and last point, because the they are always 0 and therefore have the second derivative 0. However, the end-points can still be used to calculate the second derivative, although they are not in the correlation-matrix, since it is 0.

Taking the derivative or finding the velocity in 1 dimension of the wave-function is done numerically using [5, eq. 5.4]

$$\nabla u_i = \frac{u_{i+1} - u_{i-1}}{2\Delta}. \quad (3.9)$$

The effective potential $V_e(s)$ only acts on the point itself. Therefore it will have to be added along the diagonal of the correlation-matrix. This is the only part of the matrix which changes in the four Hamiltonian operators.

Now that the correlation-matrix is created the eigenvalues and eigenvectors can be found by using the routine `gsl_eigen_nonsymm` in GNU Scientific Library. The physical meaning of eigenvalue is the energy of the state. The physical meaning of eigenvector is the wave-function, where each element of eigenvector is the wave-function in corresponding element i \vec{u} . After sorting for the lowest eigenvalue and then in increasing order it is known which is the ground state, first excited state and so on.

Then by returning the eigenvector elements to their corresponding points on the line the wave-function of the state is found.

An example of wave-function of the ground state for the first Hamiltonian operator can be seen at Figure 3.1.

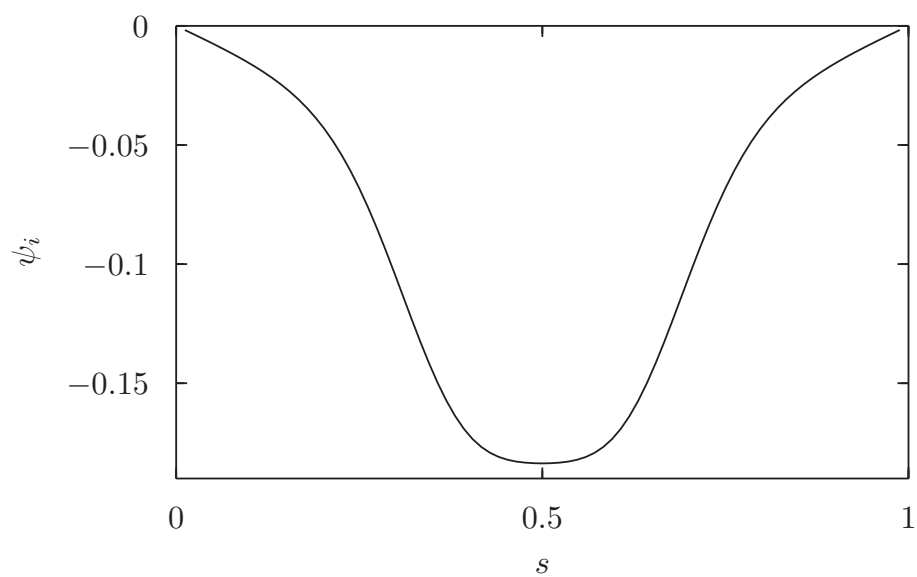


Figure 3.1: *The wave-function of the ground state for the first Hamiltonian operator.*

Chapter 4

Method for Comparison of the different systems

To compare the 2-dimensional simulation to the 1-dimensional derived Hamiltonian operators they must be based in the same coordinate system. It is chosen in this thesis to compare in the x-coordinates. Because of this choice there must be a change of coordinates from 1-dimensional s-coordinates to x-coordinates as used in the simulation.

4.1 Change from s-coordinates to x-coordinates

The probability that the particle is in the interval from $s - \Delta/2$ to $s + \Delta/2$ is given by [4, eq. 1.3]

$$P_s(s - \Delta, s + \Delta) = \int_{s-\Delta/2}^{s+\Delta/2} |\psi(s)|^2 ds \quad (4.1)$$

S-coordinates is the 1-dimensional coordinate that follows the lowest point in simulated potential which, as mentioned earlier, in this case is the Gauss function

$$f(x) = A + B e^{-(x-L/2)^2/a^2}. \quad (4.2)$$

To make the change from s-coordinates to x-coordinates the following formula is used, where y is given by the function for lowest potential:

$$ds^2 = dx^2 + dy^2 \quad (4.3)$$

$$\begin{aligned} ds &= \sqrt{dx^2 + dy^2} \\ &= \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx \end{aligned} \quad (4.4)$$

This is then used make the change form s-coordinates to x-coordinates, which gives the probability

$$P_x(s(x)) = \int_{s(x)-\Delta/2}^{s(x)+\Delta/2} |\psi(s(x))|^2 \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx. \quad (4.5)$$

When this is calculated numerically for each point, the point is at the centre of the interval. Whereby $\psi(s)$ is assumed to be the average value of the interval. This method is known as trapezoidal approximation [6]. The first and the last point at $s(x) = 0$ and $s(x) = L$ will only have half the interval, however they have to fulfil $\psi = 0$ since the wave-function cannot leave the 1-dimensional box. The probability is then calculated by

$$P_x(s(x)) = \Delta |\psi(s(x))|^2 \sqrt{1 + \left(\frac{dy}{dx}\right)^2}. \quad (4.6)$$

To make it easier to compare the probability-functions they are normalised, which is done by adding all values together and divide each value by the total value, whereby Δ can be reduced since all interval have the same size

$$P_x(s(x)) \propto |\psi(s(x))|^2 \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx. \quad (4.7)$$

4.2 Analytical sine-function

The solutions for a 1-dimensional box is well known to be a sine-function [4, eq. 2.28]. Therefore also an analytical sine-function in s-coordinate along with the four Hamiltonian operators is included. This analytical sine-function in s-coordinate has to go through the exact same coordinate change to x-coordinates, whereby the probability of the normalised analytical sine-function is

$$P_x(s(x)) \propto |\sin(cs(x))|^2 \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx, \quad (4.8)$$

where c determines which state the wave-function is in and the sine-function has to start and end at 0. If c is 1, then it is the ground state, for c higher than one it is the $c - 1$ excited state.

4.3 Making the simulation comparable

The simulation is already in the x-coordinate, whereby there is no need for a change for coordinates. The probability that the particle is in the given area is [4, eq. 1.3]

$$P_{xy}(x - \Delta, x + \Delta; y - \Delta, y + \Delta) = \int_{s-\Delta/2}^{s+\Delta/2} \int_{y-\Delta/2}^{y+\Delta/2} |\psi(x, y)|^2 dy dx. \quad (4.9)$$

When this is calculated numerically for each point, the point is at the centre of the area. Whereby $\psi(x, y)$ is assumed to be the average value of area [6]. The points on the side of the plane will have half or quarter of the area, however, they have to fulfil $\psi = 0$ since the wave-function cannot leave the 2-dimensional box. The probability is then calculated by

$$P_{xy}(x; y) = \Delta^2 |\psi(x, y)|^2. \quad (4.10)$$

To get the probability for x and not for each individual x,y pair, all values of y for a given x are added up, which give

$$P_x(x) = \Delta^2 \sum_y |\psi(x, y)|^2. \quad (4.11)$$

To make it easier to compare the probability-functions they are normalised, which is done by adding all values together and divide each value by the total value, whereby Δ can be reduced since all areas have the same size

$$P_x(x) \propto \sum_y |\psi(x, y)|^2. \quad (4.12)$$

Chapter 5

Results

The results is simulated with 85 points on each side, the length of the box L is 1 length unit, the constant k is set to 1000 energy units per length unit squared, the height of the Gauss function B is 0.39 length unit, the starting height of the Gauss-function A is determined by the length of the box and the height of the Gauss function, whereby it is 0.305 length unit, a which controls the width of the Gauss function is set to 0.25 length unit, the mass m is 1 mass unit, and \hbar is chosen to have the value 1 energy unit times time unit.

All probability-distributions for the ground state can be seen in Figure 5.1. The first thing one notes is that the overall shape of the simulation (Black) and the Hamiltonian operators are different. The third (Blue) and fourth (Yellow) Hamiltonian operator are close too each other. The second (red) Hamiltonian operators is closest to the analytical sine-function (Orange). The Hamiltonian operator which is closest to the simulation is the first (Green) Hamiltonian operator though the first Hamiltonian operator is wider and has a lowering in the middle of the probability-distribution.

All the probability-distributions for the first excited state in one figure can be seen in Figure 5.2. The first thing which springs to mind is that the overall shape of the simulation (Black) and the Hamiltonian operators are not different. The height and with of the probability-distributions look similar though the tops of the probability-distributions shifted between the simulation (Black) and the analytic sine-function (orange). The third (Blue) and fourth (Yellow) Hamiltonian operators are so close too each other that it is hard to say which is closer to the simulation. This time the first (Green) and second (Red) Hamiltonian operators are similar to the third and fourth just a bit longer away from the simulation.

Al the probability-distributions for the second excited state can be seen in one figure Figure 5.3. It is clear that the overall shape of the simulation (Black) and the Hamiltonian operators are somewhat different. The third (Blue) and fourth (Yellow) Hamiltonian operator are close to each other again and they are both too small in the first third, too large and have a lowering in the middle, and too small in the last third. This time the first (Green) and second (Red) Hamiltonian operators is closer to the simulation each in different parts, where the second Hamiltonian operator is closer in the first and last thirds of the simulation and first Hamiltonian operator is closer in the middle of simulation.

The probability distributions for the third excited state can be seen in

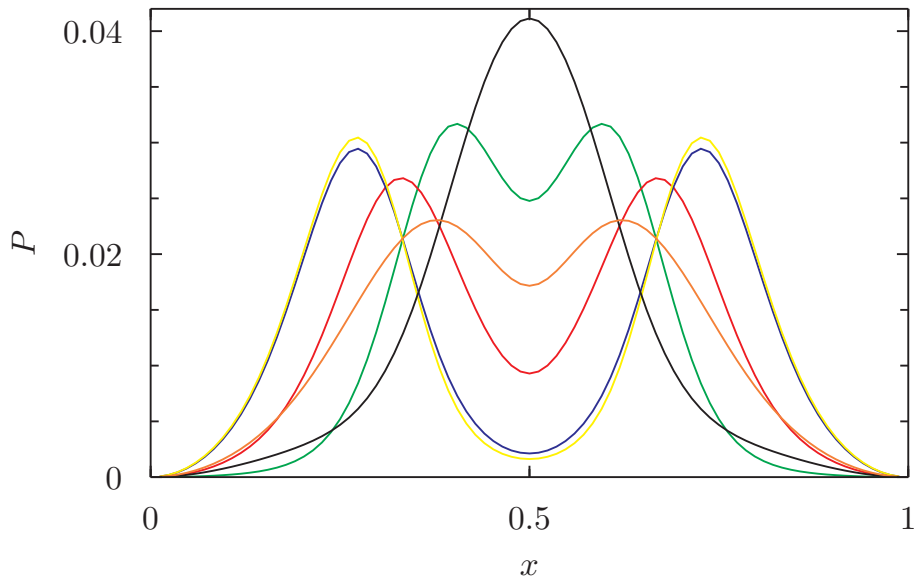


Figure 5.1: All the probability distributions for the ground state plotted together. The black line is the simulation, the orange line is the analytical sine-function, the green line is the first Hamiltonian operator, the red line is the second Hamiltonian operator, the blue line is the third Hamiltonian operator and the yellow line is the fourth Hamiltonian operator.

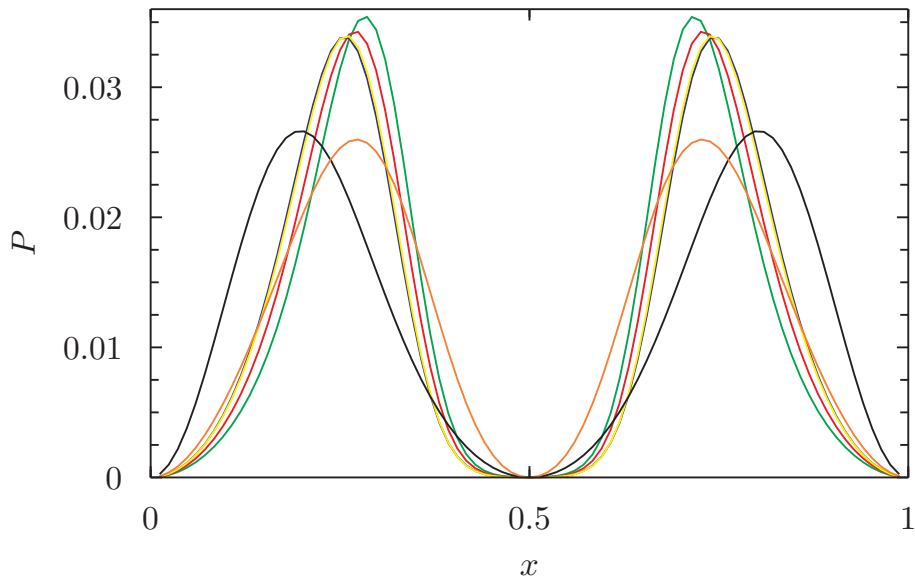


Figure 5.2: All the probability distributions for the first excited state plotted together. The black line is the simulation, the orange line is the analytical sine-function, the green line is the first Hamiltonian operator, the red line is the second Hamiltonian operator, the blue line is the third Hamiltonian operator and the yellow line is the fourth Hamiltonian operator.

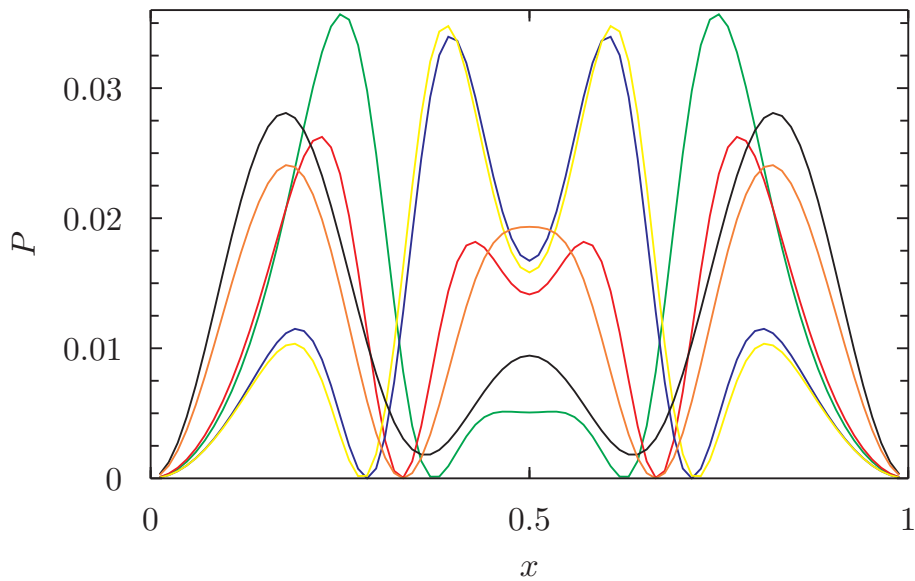


Figure 5.3: All the probability distributions for the second excited state plotted together. The black line is the simulation, the orange line is the analytical sine-function, the green line is the first Hamiltonian operator, the red line is the second Hamiltonian operator, the blue line is the third Hamiltonian operator and the yellow line is the fourth Hamiltonian operator.

Figure A.1 and for fourth excited state in Figure A.2 in the appendix, however they are not included in the results since they are not giving any additional insight.

Chapter 6

Discussion

6.1 Interpretation of the results

In the results it can be seen that the third and fourth Hamiltonian operators follow each other closely. This can be explained by the little difference them

$$\hat{H}_3 - \hat{H}_4 = -\frac{\hbar^2}{2} \frac{1}{4} \frac{m'(s)^2}{m(s)^3}. \quad (6.1)$$

Based on the results none of the four Hamiltonian operators is better over all states than the others, whereby none of them can be the correct position-dependent effective mass Hamiltonian operator for the position-dependent effective mass Schrödinger equation.

According to [2, section 4] all other Hamiltonian operators than the one, in this thesis called the first Hamiltonian operator, can not be the correct Hamiltonian operator since any other Hamiltonian operator is not consistent with the continuity condition in the case the mass is discontinuous.

If both this result and the simulation in this thesis are correct, the result is that there is no position-dependent effective mass Hamiltonian operator.

6.2 Errors from the numerical method

Since the calculations made in this thesis are calculated numerically they will not be precise. For the second derivative error is given [5, page 3]

$$-\frac{\Delta^2}{12} \psi''''(\xi). \quad (6.2)$$

and for the first derivative error is given [5, eq. 5.5]

$$-\frac{\Delta^2}{6} \psi''''(\xi) \quad (6.3)$$

where ξ is a value between $s - \Delta$ and $s + \Delta$ such that the wave-function at ξ is the average of the wave-functions at $s - \Delta$ and $s + \Delta$. For the simulation there is a second derivative error in both the x- and y-directions. For the numerical integration using the trapezoidal rule there is also a error [6]

$$\frac{\Delta^3}{12} P''(x). \quad (6.4)$$

Since the analytical wave-function and probability-distribution not are known, it is not possible to calculate the error, however, the factors in front of wave-function and probability-distribution can be calculated to give an idea of the size of the error. In this thesis there is used 85 points and a length of 1 then Δ becomes $1/84$. The factor in front of the second derivative is $-1/84672$, for the first derivative $-1/42336$, and on the integration $1/7112448$. These number are quit small even when multiplied by the wave-function or the probability-distribution, whereby they can be approximated to neglectable.

6.3 Futher work

If further work has to be done based on this thesis the best way to improve it is to expand the number of Hamiltonian operators used for comparison. This can be done by taking the generalized Hamiltonian operator without a potential [2, eq. 3.19]

$$\hat{H}_g = P \frac{1}{2M} P + \frac{1}{2} (\alpha + \gamma + \alpha\gamma) \frac{M'^2}{M^3} - \frac{1}{4} (\alpha\gamma) \frac{M''}{M^2} \quad (6.5)$$

and having a program trying different values for α , β , and γ and comparing with the simulation to find the best comparison values.

An alternative way is to change the Gauss function to some other function which still meets the conditions and see whether this changes any of the results.

Chapter 7

Conclusions

In this thesis numerical methods were used to make a 2-dimensional simulation of the position-dependent effective mass using an built-in potential to increase the length the particle have to travel corresponding to the increasing mass.

Four Hamiltonian operators were chosen to be compared to the 2-dimensional simulation. Each of these four Hamiltonian operators were written out, so that it could be put in its own 1-dimensional box. In these 1-dimensional boxes there were no potentials, the Hamiltonians operators themselves, however, had an effective potential.

After changing coordinates and calculating the probability-distributions, it could be found which of the four Hamiltonian operators had the best correspondence to the simulation. For the ground state the Hamiltonian operator corresponding best was the first. For the first excited state the Hamiltonian operators corresponding best were the third and fourth, since they were so close together that it was not possible to tell which was the better. For the second excited state the Hamiltonian operator corresponding best was the second in the first and last third, while the first Hamiltonian operator corresponded best to simulation in the middle.

Because no single of the four Hamiltonian operators corresponds to the simulation, there is not found a single Hamiltonian operator that can represent the position-depended effective mass equation.

There are two different ways of expanding on this work. The first is to increase the number of Hamiltonian operators since this thesis has only tested four of the infinitely many Hamiltonians. An alternative is to investigate whether the results are the same if the function changes to someting different from a Gauss function.

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Appendix A

The probability-distribution for third and fourth excited state

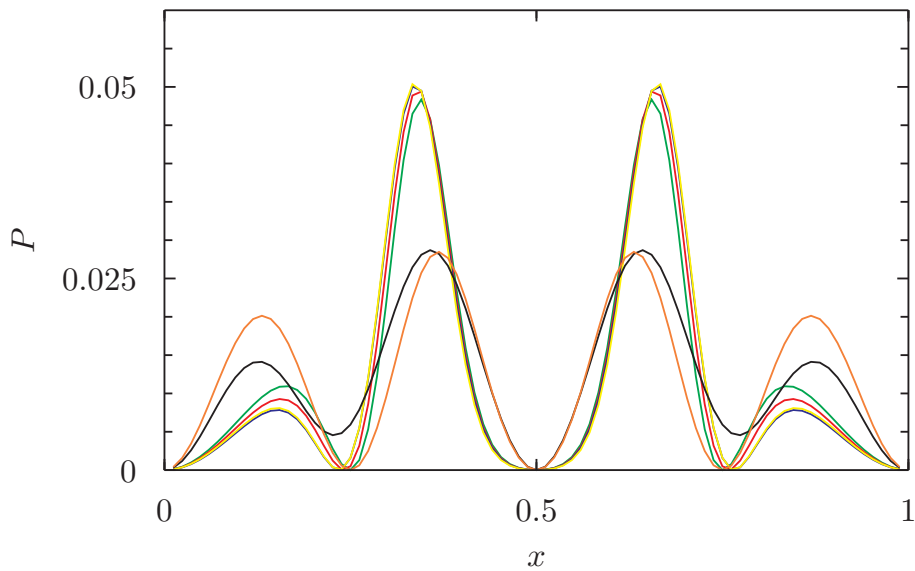


Figure A.1: All the probability distributions for the third excited state plotted together. The black line is the simulation, the orange line is the analytical sine-function, the green line is the first Hamiltonian operator, the red line is the second Hamiltonian operator, the blue line is the third Hamiltonian operator and the yellow line is the fourth Hamiltonian operator.

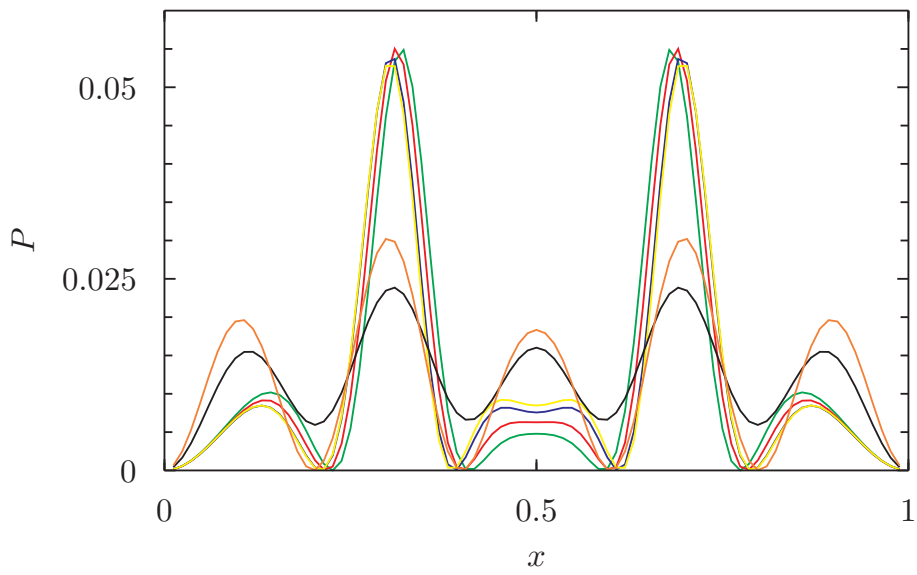


Figure A.2: All the probability distributions for the fourth excited state plotted together. The black line is the simulation, the orange line is the analytical sine-function, the green line is the first Hamiltonian operator, the red line is the second Hamiltonian operator, the blue line is the third Hamiltonian operator and the yellow line is the fourth Hamiltonian operator.