A classical particle in a quantum box

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July 15, 2009

Abstract

Coherent states in a harmonic oscillator describe systems that are in a quasiclassical state. The purpose of this article is to find out if this also applies to an infinite square well. Herefore two different approaches are used: The first approach creates the coherent function in the position representation and takes the limit for a high expectation value for the energy of the system. The resulting function shows classical behavior. However it still complies to Heisenberg‘s principle and has a certain uncertainty in position and momentum which increases in time. In the second approach the expectation value of the position of a coherent function is analyzed in the limit for high energies. Here we see with the use of Fourier transformation that it converges towards a sawtooth function. Consequently with this approach we can again conclude that there is classical behavior. The final result is that a quasiclassical state can be created in an infinite quantum square well. However the resulting state will not keep minimal uncertainty under time evolution like a coherent state in a harmonic oscillator.

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1 Introduction

The subject of research in this article is the rather simple system of a particle in a box. Classically the movement of such a particle, assuming that it has no interaction with the outer world, is very intuitive and trivial. If Newton's laws of motion are applied the particle will move with uniform velocity in straight lines until it reflects from a wall. However in quantum physics there is a very different approach: the Schrödinger equation. This will lead to a description of the particle as a linear combination of the eigenfunctions of the Schrödinger equation belonging to the system. In addition these solutions to the problem do not seem to have anything in common with the classical ones. However in this article we will survey the coherent state - a special type of quantum state - that should result in a behavior closest to the classical movement of a particle.

The purpose of this article will be to show that the mathematical definition of a coherent state and the resulting wavefunction will yield a quantum state that shows classical behavior. Therefore we expect this state to move uniformly and to have negligible uncertainty in position and momentum. For this purpose we will use two different approaches. In the first approach (chapter 3) we will create the coherent wavefunction from the definition of coherent states. Then, after different simplifications, the expression for the wave function shall converge to a 'classical' function. The second approach (chapter 4) will make use of Fourier transformations. Here we will try to show that the expectation value of the observable of the position x will have the same Fourier transformation as the 'sawtooth function', which will imply that also both functions are equal. The consequence is that the expectation value of the position becomes classical.

When speaking of a classical system we make the a priori assumptions that the uncertainties in position and momentum are zero. Thus the behavior of the system is entirely determined. In contrast this is not possible for a quantum mechanical system that obey the Heisenberg uncertainty principle. Therefore it is not possible to create an entirely classical system by a quantum mechanical approach. However we can create a state that is as classical as possible, meaning that uncertainty in position and momentum is minimal. Such a state is called a coherent state.

For the definition of the coherent state we will make use of the Dirac Notation. A good introduction to this formalism can be found in 'Introduction to Quantum Mechanics' by David J. Griffith [1]. In addition this book introduces the infinite square well and the concept of ladder operators which belong to the background of this article. However we will construct the raising operator in a more general way that this is done in Griffith's book.

2 Theoretical Background/Coherent Quantum States

2.1 A particle in a box

The theory of a particle in a box or an infinite square well will be the basis for this article. As it is not the purpose of this article to derive the eigenstates and eigenenergies we will only introduce them here. A detailed derivation can be found in 'Introduction to Quantum Mechanics' by David J. Griffith's [1]. To describe an infinite square well we will use the following potential:

$$\hat{V} = \begin{cases} \infty & \text{if } x < 0 \\ 0 & \text{if } 0 < x < L \\ \infty & \text{if } L < x \end{cases} \tag{1}$$

The time-independent solutions $\psi_n(x)$ for the appertaining Schrödinger equation

$$\hat{H}\psi = E\psi \text{ with } \hat{H} = \frac{\hat{p}^2}{2m} + \hat{V} \tag{2}$$

are given by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \tag{3}$$

The corresponding eigenenergies E_n which are the eigenvalues of the Hamiltonian are:

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2 \tag{4}$$

Going over to Dirac-notation the eigenfunctions in position representation are defined by:

$$\langle x|n\rangle = \langle x|\psi_n\rangle = \psi_n(x) \tag{5}$$

A time-dependent solution to the Hamiltonian can be created by adding a time evolution to the time-independent solutions:

$$|n\rangle \rightarrow |n\rangle e^{-iE_n t/\hbar} \tag{6}$$

These functions form a complete orthogonal set. As a result any state $|\psi\rangle$ describing our system can be formed by lineair combinations of these wavefunctions:

$$|\psi\rangle = \sum_{n\in\mathbb{N}} c_n |n\rangle e^{-iE_n t/\hbar} \tag{7}$$

For normalizations reasons, $\langle\psi|\psi\rangle = 1$, we get the following equation for the expansion coefficients c_n

$$1 = \sum_{n\in\mathbb{N}} |c_n|^2 \tag{8}$$

2.2 Coherent quantum states

2.2.1 Lowering and raising operators

To define a coherent state we make use of the lowering operator $\hat{a}$.

For a quantum system like the infinite square well, that has an infinite number of non-degenerate normalized energy eigenstates $\{|n\rangle;\ n = 0, 1, 2, ..\}$, we can define the lowering operator by:

$$\hat{a} = \sum_{n\geq 0} \sqrt{n+1}|n\rangle\langle n+1| \tag{9}$$

For this operator we can derive the following properties that will be used to define the coherent state:

The lowering operator $\hat{a}$, working on an energy eigenstate, lowers the state by one:

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \tag{10}$$

And it returns zero working on the ground state:

$$\hat{a}|0\rangle = 0|0\rangle \tag{11}$$

The lowering operator and its conjugate operator $\hat{a}^\dagger$, the raising operator given by

$$\hat{a}^\dagger = \sum_{n\geq 0} \sqrt{n+1}|n+1\rangle\langle n| \tag{12}$$

do not commute. Their products are

$$\begin{aligned} \hat{a}\hat{a}^\dagger &= \sum_{n,n'\geq 0} \sqrt{(n+1)(n'+1)}|n\rangle\langle n+1|n'+1\rangle\langle n'| \\ &= \sum_{n\geq 0}(n+1)|n\rangle\langle n|, \\ \hat{a}^\dagger\hat{a} &= \sum_{n,n'\geq 0} \sqrt{(n+1)(n'+1)}|n+1\rangle\langle n|n'\rangle\langle n'+1| \\ &= \sum_{n\geq 1} n|n\rangle\langle n| = \sum_{n\geq 0} n|n\rangle\langle n| \end{aligned} \tag{13}$$

Therefore the commutator is:

$$[\hat{a}, \hat{a}^\dagger] = \sum_{n\geq 0} |n\rangle\langle n| = \hat{1} \tag{14}$$

This commutation relation is the property that defines $\hat{a}$ and $\hat{a}^\dagger$ to be lowering and raising operators.

2.2.2 Introduction of the coherent state

Now we can define a coherent state. Mathematically, a coherent state $|\alpha\rangle$ is defined as an eigenstate of the lowering operator $\hat{a}$. Formally, this reads:

$$\hat{a}|\alpha\rangle = s|\alpha\rangle \tag{15}$$

Here the eigenvalue s is in general a complex number for $\hat{a}$ is not Hermitian.

A coherent state can be expanded in terms of energy eigenstates just like any other wave function:

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n|n\rangle \tag{16}$$

To determine the expansion coefficients let the lowering operator work on the coherent state:

$$\hat{a}|\alpha\rangle = \sum_{n=0}^{\infty} c_n\hat{a}|n\rangle \overset{(11)}{=} \sum_{n=1}^{\infty} c_n\sqrt{n}|n-1\rangle = \sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle \tag{17}$$

As coherent states are eigenfunctions of $\hat{a}$ (equation (15)) we know that this state will only differ by a factor s from the coherent state we began with. Thus:

$$\sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle = s\sum_{n=0}^{\infty} c_n|n\rangle \tag{18}$$

The energy eigenstates are orthonormal and therefore we get:

$$c_{n+1}\sqrt{n} = c_n s \quad \forall n = 0, 1, 2... \tag{19}$$

This yields the following expression for the expansion coefficients.

$$c_n = \frac{s}{\sqrt{n}}c_{n-1} = ... = \frac{s^n}{\sqrt{n!}}c_0 \tag{20}$$

Finally to determine c_0 we normalize our state. With the normalization condition (8) we get:

$$1 = |c_0|^2 \sum_{n=0}^{\infty} \frac{(|s|^2)^n}{n!} \tag{21}$$

Where the sum is the polynomial expansion of the natural exponent. Thus we can write:

$$1 = |c_0|^2 e^{|s|^2} \tag{22}$$

Solving for c_0 yields:

$$c_0 = e^{\frac{-|s|^2}{2}} e^{i\theta} \tag{23}$$

There is no physical meaning for the complex phase θ of c_0. It is just an overall factor for all c_n and therefore there is no influence on $|\alpha|$. Hence, to keep it simple we choose $\theta = 0$ and so we arrive at the following equation for the expansion coefficients of a coherent state:

$$c_n = e^{-\frac{|s|^2}{2}} \frac{s^n}{\sqrt{n!}} \tag{24}$$

Figure 1 shows c_n as a function of n. Here the similarity to a Gaussian function is easy to see. This property will be used later on in the classical limit.

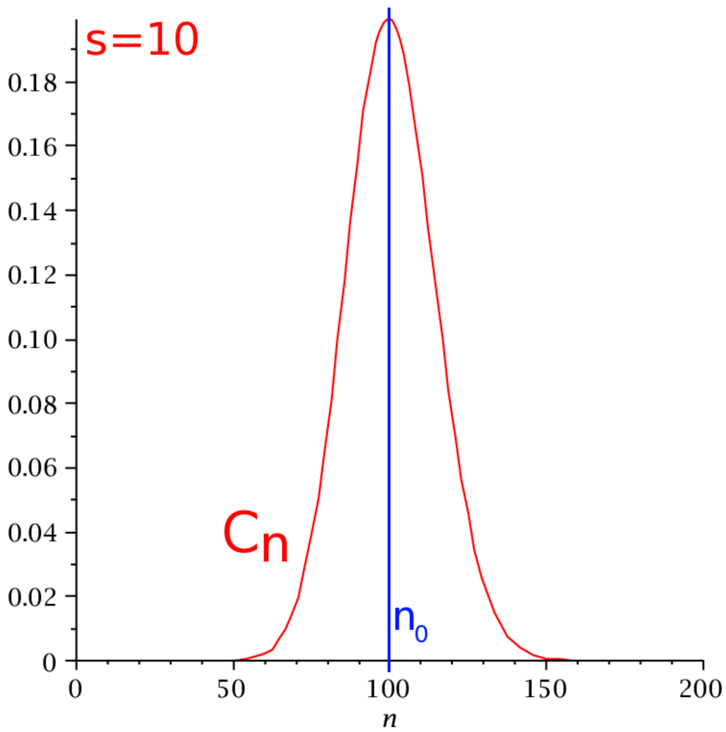

Figure 1: Here we see c_n with eigenvalue $s = 10$

2.2.3 Time-dependent coherent states

What will happen to the coherent state if we put in the time-dependence?

$$|n\rangle \rightarrow e^{-iE_n t/\hbar}|n\rangle$$

The coherent function becomes:

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n e^{-iE_n t/\hbar}|n\rangle \tag{25}$$

And thus the eigenvalue equation for coherence changes to

$$\begin{aligned}
&\hat{a}|\alpha\rangle = s|\alpha\rangle \\
\Leftrightarrow &\sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}e^{-iE_{(n+1)}t/\hbar}|n\rangle = s\sum_{n=0}^{\infty} c_n e^{-iE_n t/\hbar}|n\rangle \\
\Leftrightarrow &\sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}e^{-iE_n t/\hbar}|n\rangle e^{-i\Delta E t/\hbar} = s\sum_{n=0}^{\infty} c_n e^{-iE_n t/\hbar}|n\rangle
\end{aligned}$$

Where

$$\Delta E = E_{n+1} - E_n = \frac{\pi^2\hbar^2}{2mL^2}(2n+1) \tag{26}$$

Since ΔE is a function of n it is not possible to find an eigenvalue s so that this equation holds for constant c_n's. Consequently equation (15) will only hold for $t = 0$. For $t > 0$ the eigenfunctions will run out of phase, because of the extra phase factor $e^{-i\Delta E(n)t/\hbar}$. Hence the 'coherent function' will become less coherent during its evolution in time. This means for a coherent state in a box that its wave function will spread out as time goes by.

This stands in contrast to the coherent states of the harmonic oscillator which stay coherent (see appendix A). Here the energy eigenvalues $E = \hbar\omega(n + \frac{1}{2})$ are equidistant and so the phase factor $e^{-i\Delta E t/\hbar}$ can be extracted from the sum and the following time-dependent equation for the eigenvalue of the coherent state can be derived:

$$s(t) = e^{-i\Delta E t/\hbar}s \tag{27}$$

In addition it is rather simple to derive the expectation values of position and momentum using ladder operator. That makes it possible to show that the state has minimal uncertainty (see appendix A). However for a quantum well with infinite walls we cannot express position and momentum easily with ladder operators. Therefore we will use a different approach to show that the wave function shows classical behavior. In the following two chapters we will try to show in two different ways that also in an infinite square well a coherent state is the most classical state possible.

3 Classical limit

3.1 Preparations

The function we are going to approximate is the coherent state:

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle e^{-iE_n t/\hbar} \tag{28}$$

where c_n is given by equation (20).

As we want to get an expression that is more compact and that gives more insight into the behavior of the state we need to make several approximations. The purpose will be to come to a function that is not a sum over n anymore. We will see later on that the sum can be approximated by an integral.

First we will determine the position of the maximum of c_n. This lies at the place where the growth of the factorial $\sqrt{n!}$ in the denominator exceeds the the growth of the power s^n. Thus we can regard successive values of c_n for they have to be almost equal at the maximum. We write:

$$1 \approx \frac{c_{n_0+1}}{c_{n_0}} = \frac{s^{n_0+1}}{\sqrt{(n_0+1)!}} \frac{\sqrt{n_0!}}{s^{n_0}} = \frac{s}{\sqrt{n_0}} \tag{29}$$

Consequently the maximum lies at:

$$n_0 = |s|^2 \tag{30}$$

It is true that the maximum does not lie precisely at n_0, but in between n_0 and $n_0 + 1$. However this will be negligible for the further process.

To be able to speak of a classical particle it must not be affected by the discreteness of the eigenenergies. Hence we expect a classical particle to have a high probability of finding it in energy eigenstates with high energies. These have less discernible energy transition and for large n we can speak of an almost continuous spectrum. Therefore in a classical state we also want the maximum of the c_n coefficients to correspond with a high energy eigenstate. This means that n_0 and consequently s have to be big. To make a long story short: to create a classical situation with coherent states we have to chose the eigenvalue s of $\hat{a}$ large.

To give the reader a feeling of the size of s we can make a simple calculation: Take a billiard ball with a mass of $m = 160g$ and velocity $v = 10\frac{m}{s}$ the kinetic energy of this ball is:

$$E_{kin} = \frac{1}{2}mv^2 = 8J \tag{31}$$

If we want to describe a particle with these properties in the quantum well, it has to have the same energy expectation value, which is:

$$E_{n_0} = \frac{\pi^2\hbar^2}{2mL^2}n_0^2 \tag{32}$$

We will see later on that c_n can be approximated by a Gaussian function symmetric around n_0. Therefore n_0 will also be the expectation value for the energy eigenstate. Solving equations (31) and (32) for n_0 yields:

$$n_0 = \frac{L}{\pi\hbar}\sqrt{2mE} = \frac{L}{\pi\hbar}mv = 4.8 \cdot 10^{33} \tag{33}$$

For a classical system we can expect L,m and v to be at orders of $1m$, $1kg$ and $1m/s$ respectively. Hence we can assume that

$$n_0 = \mathcal{O}(\frac{Js}{\hbar}) \tag{34}$$

for a classical system. Consequently we can say that

$$|s| = \mathcal{O}(\sqrt{\frac{Js}{\hbar}}) \tag{35}$$

Thus taking the classical limit of a particle in a box means to create a coherent state and let the absolute value of the eigenvalue s become of order of $\sqrt{\frac{Js}{\hbar}}$.

c_n goes to zero for $n \ll n_0$ and $n \gg n_0$. Hence we will expect that the energy eigenfunction that determine the properties of $|\alpha\rangle$ will lie around the maximum at n_0. Therefore we will substitute n with

$$n(k) = n_0 + k \tag{36}$$

whereas k will become the new parameter to sum over. With this we put the focus on the eigenfunction that are of importance for the behavior of the wave function.

3.2 The expansion coefficient c_n for large n

First we write s in exponential form. We will see later on that with (30) this will simplify the expression a lot.

$$s^n = (|s|e^{i\phi})^n = |s|^n e^{i\phi n} \text{ with } \phi = \arg(s) \tag{37}$$

Plugging this into the expansion coefficient yields:

$$c_n = e^{-\frac{|s|^2}{2}} \frac{|s|^n e^{i\phi n}}{\sqrt{n!}} \tag{38}$$

However there are more possibilities to write the expansion coefficients. We can make the following substitution for the complex phase

$$\phi \rightarrow \phi + 2\pi j \text{ with } j \in \mathbb{Z} \tag{39}$$

With this c_n will become “dependent” on the new parameter j:

$$c_n \rightarrow c_{n,j} = e^{-\frac{|s|^2}{2}} \frac{|s|^n e^{i(\phi+2\pi j)n}}{\sqrt{n!}} \tag{40}$$

It is true that the complex phase or the absolute value of the expansion coefficients is not changed in any way.

So why would we make the expression more complicated than it already is? During the further calculations we will need to complete a square in the exponent of the expression of the wave function. This will mean that real terms and imaginary terms in the exponent will be “mixed”. Consequently also the initial complex phase of c_n will have a contribution to the absolute value of the wave function. Taking a different j will result in a different wave function. Therefore every j will correspond with a different part of the total wave function that is a solution to our system. Hence we will construct the total coherent wave function $|\alpha\rangle$ by summing over all solutions $|\alpha_j\rangle$ belonging to different j's.

$$|\alpha\rangle = \sum_j |\alpha_j\rangle \tag{41}$$

We will approximate c_n around the maximum at n_0, due to the fact that here will find the eigenstates with the biggest contribution to the coherent state.

As we take n_0 large we can use Stirling's approximation for factorial's of large numbers

$$n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \tag{42}$$

to eliminate the factorial in the denominator.
Substitution yields:

$$c_n = \frac{e^{-\frac{|s|^2}{2}}}{(2\pi)^{1/4}}\frac{1}{n^{1/4}}\left(\frac{e}{n}\right)^{n/2}|s|^n e^{i(\phi+2\pi ij)n} \tag{43}$$

It will become useful to write all terms dependent on n in one exponent:

$$c_n = \frac{e^{i\Phi_j(n)}}{(2\pi)^{1/4}}e^{-\frac{|s|^2}{2}+\frac{n}{2}+n\ln|s|-\frac{1}{2}(n+\frac{1}{2})\ln(n)} \tag{44}$$

Here we used

$$\Phi_j(n) = (\phi + 2\pi j)n \tag{45}$$

to collect the complex phase in one variable. However keep in mind that this phase is still a function of n and j.

Using (36) to substitute n and (30) to substitute $|s|$ we arrive at the following expression:

$$c_{n_0+k} = \frac{e^{i\Phi_j(n)}}{(2\pi)^{1/4}}e^{\frac{k}{2}+\frac{1}{2}(n_0+k)\ln(n_0)-\frac{1}{2}(n_0+k+\frac{1}{2})\ln(n_0+k)} \tag{46}$$

Expanding $\ln(n_0+k)$ in a Taylor series

$$\ln(n_0+k) = \ln(n_0) + \frac{k}{n_0} - \frac{k^2}{2n_0^2} + ... \tag{47}$$

the last term of the exponent becomes:

$$-\frac{1}{2}\left((n_0+k)\ln(n_0) + \frac{1}{2}\ln(n_0) + k + \frac{k^2}{n_0} + \frac{k}{2n_0} - \frac{k^2}{2n_0}\underbrace{-\frac{k^3}{2n_0^2} - \frac{k^2}{4n_0^2} + ...}_{\text{negligible}}\right) \tag{48}$$

We will neglect those terms that are at least a factor n_0 smaller than other terms with the same power of k. Furthermore we will neglect all terms with a power of k greater than 2. We do this because we expect that $k \ll n_0$ for all important eigenstates around the maximum.

The expression for the expansion coefficients becomes:

$$c(k) \equiv c_{n_0+k} = \frac{e^{i\Phi_j(n)}}{(2\pi n_0)^{1/4}} e^{-\frac{1}{4n_0}(k^2+k)} \tag{49}$$

Completing the square in the exponent yields:

$$c(k) = \frac{e^{i\Phi_j(n)}}{(2\pi n_0)^{1/4}} e^{-\frac{1}{4n_0}((k+\frac{1}{2})^2-\frac{1}{4})} \tag{50}$$

Now we can see that the absolute value of this function is a Gaussian function with the following expectation value and uncertainty:

$$\mu_{c(k)} = -\frac{1}{2} \tag{51}$$

$$\sigma_{c(k)} = \sqrt{2n_0} = \sqrt{2}|s| \tag{52}$$

The expectation value still tells us that the maximum lies somewhere between n_0 and n_0+1. This is of minor value to us, we already assumed this beforehand. However the uncertainty points out that it is reasonable to neglect terms that have higher order than $|s|$. Thus in the following we will assume that:

$$k = \mathcal{O}(|s|) = \mathcal{O}(\sqrt{n_0}) \tag{53}$$

It is easy to prove that the coefficients are still normalized in the classical limit:

$$\int dk|c(k)|^2 = \frac{e^{\frac{1}{8n_0}}}{\sqrt{2\pi n_0}} \int dk e^{-\frac{(k+\frac{1}{2})^2}{2n_0}} = \frac{e^{\frac{1}{8n_0}}\sqrt{2\pi n_0}}{\sqrt{2\pi n_0}} = e^{\frac{1}{8n_0}}$$

For $n_0 = \mathcal{O}(\frac{Js}{\hbar})$ we can approximate $e^{\frac{1}{8n_0}}$ with 1.

3.3 Derivation of the expression for $|\alpha\rangle$ in the classical limit

With equations (34) and (36) we can say that a small variation in k ($k \to k \pm 1$) will lead to a minimal variation in $n(k)$. Thus it seems to be legitimate to handle $n(k)$ as a real parameter. This comes in handy, because then we can approximate the sum over n with an integral over k.

In addition due to the fact that the limit of $c(k)$ to $\pm\infty$ is zero it will not be noticeable in the result, if the lower integration boundary is $k = -\infty$ in place of $k = -n_0$. Therefore we can approximate the sum in the following manner:

$$|\alpha_j\rangle = \sum_{n=0}^{\infty} c_n |n\rangle e^{-\frac{i\hbar\pi^2 n^2 t}{2mL^2}} \overset{n=n_0+k}{\approx} \int_{k=-\infty}^{\infty} dk \;\; c(k)|n_0+k\rangle e^{-\frac{i\hbar\pi^2(n_0+k)^2 t}{2mL^2}} \tag{54}$$

Going over to $\alpha_j \equiv \alpha_j(x,t) = \langle x|\alpha_j\rangle$ we get the following expression:

$$\alpha_j = \int_{k=-\infty}^{\infty} dk \;\; \frac{e^{i\Phi_j(n_0+k)}}{(2\pi n_0)^{1/4}} e^{-\frac{1}{4n_0}(k^2+k)} \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} e^{-\frac{i\hbar\pi^2(n_0+k)^2 t}{2mL^2}} \tag{55}$$

Using the substitution $\sin x = \frac{1}{2i}(e^{ix} - e^{-ix})$ we can rewrite this to an integral over two exponents:

$$\alpha_j = A \int_k dk \quad \left[e^{F_j(k,x,t)} - e^{F_j(k,-x,t)} \right] \tag{56}$$

where A and the function F_j can be derived from the original wavefunction:

$$A = (2\pi n_0)^{-1/4} \frac{1}{2i} \sqrt{\frac{2}{L}} \tag{57}$$

$$F_j(k,x,t) = \underbrace{-\frac{(k^2+k)}{4n_0} + i\Phi_j(n_0+k)}_{c(k)\text{ term}} + \underbrace{\frac{i(n_0+k)\pi x}{L}}_{\langle x|n\rangle)\text{ term}} - \underbrace{\frac{i\hbar\pi^2(n_0+k)^2 t}{2mL^2}}_{\text{time propagator term}} \tag{58}$$

Now we will write the function F_j as a polynomial of k:

$$F_j = f_{0,j} + k f_{1,j} + k^2 f_2 \tag{59}$$

with

$$f_{0,j} = i \left[(\phi + 2\pi j) n_0 - \frac{\pi^2 \hbar n_0^2 t}{2mL^2} \right] + i \frac{n_0 \pi x}{L} \tag{60}$$

$$f_{1,j} = i(\phi + 2\pi j) - \frac{1}{4n_0} + i\frac{\pi x}{L} - i\frac{\pi^2 \hbar n_0 t}{mL^2} \tag{61}$$

$$f_2 = -\frac{1}{4n_0} - i\frac{\pi^2 \hbar t}{2mL^2} \tag{62}$$

Here everything between the brackets of $f_{0,j}$ only contributes to the normalization constant. Also the dependency on t is not of importance for the properties of the wavefunction as the term only contributes to the rotation of the function in the complex plane. This will not affect the expectation value of the function. Thus we will put this term into the "constant" $K_j(t)$ to increase the readability of the equations.

$$f_{0,j} = iK_j(t) + \frac{in_0\pi x}{L} \tag{63}$$

3.3.1 Classical velocity

Let's make a substitution to give the function a more classical look. Speaking of a classical particle it will be helpful to introduce the velocity v. For this purpose we will use the classical definition of kinetic energy:

$$E_{cl} = \frac{1}{2} m v^2 \tag{64}$$

and equal it to the average energy of our system:

$$E_{n_0} = \frac{\pi^2 \hbar^2 n_0^2}{2mL^2} \tag{65}$$

this yields:

$$v = \frac{\pi \hbar n_0}{mL} \tag{66}$$

Finally our functions will look like this

$$f_{0,j} = iK_j(t) + i\frac{mvx}{\hbar}$$
$$f_{1,j} = i(\phi + 2\pi j) + \frac{i\pi x}{L} - \frac{i\pi vt}{L}$$
$$f_2 = -\frac{1}{4n_0} - \frac{i\pi vt}{2Ln_0}$$

Probably the reader will question himself where we want to end up with these approximations. The point of these calculations is to come to two exponents that have the form of a polynomial in powers of k. As we have seen in the latter approximations we neglected all terms containing k's that had a power higher than 2. The derived polynomial then can be rearranged so that we get an integral over a Gaussian function. To complete the square in the exponent we use the following expression:

$$f_2k^2 + f_{1,j}k + f_{0,j} = f_2(k + \frac{f_{1,j}}{2f_2})^2 - \frac{f_{1,j}^2}{4f_2} + f_{0,j}$$

Our wavefunction now looks in general like:

$$\alpha_j = \int_k dk \ \left(e^{a(t)(k-b)^2}\right)(e^{c_j(x,t)} - e^{c_j(-x,t)}) \tag{67}$$

Solving the integral yields:

$$\alpha_j = \sqrt{\frac{\pi}{a(t)}}(e^{c_j(x,t)} - e^{c_j(-x,t)}) \tag{68}$$

The interesting part is now the function $c_j(x,t)$ in the exponent. This function will define the movement of the particle. $c_j(x,t)$ expressed in the coefficients of the polynomial $F_j(x,t,k)$ is:

$$c_j(x,t) = -\frac{f_{1,j}^2}{4f_2} + f_{0,j} \tag{69}$$

Plugging in the three functions yields:

$$c_j(x,t) = -\frac{\pi^2 n_0}{L^2}\frac{(x - vt + \frac{\phi}{\pi}L + 2Lj)^2}{1 + 2\pi i\frac{vt}{L}} + i\frac{px}{\hbar} + iK_j(t) \tag{70}$$

Separating the imaginary part from the real part yields:

$$c_j(x,t) = -\frac{\pi^2 n_0}{L^2}\frac{(x - vt + \frac{\phi}{\pi}L + 2Lj)^2}{1 + (2\pi\frac{vt}{L})^2} \tag{71}$$
$$+ i\left[2\pi\frac{\pi^2 n_0}{L^2}\frac{(x - vt + \frac{\phi}{\pi}L + 2Lj)^2}{1 + (2\pi\frac{vt}{L})^2} + \frac{px}{\hbar} + K_j(t)\right] \tag{72}$$

Now the real part in the exponent is important for the position of the peak. The complex phase however will only play a role near the points of discontinuity of the potential, thus around $x = 0$ and $x = L$. Far away from these points, all Gaussian peaks except for one are nearly zero. Thus here the absolute value of α is only determined by the real part of the exponent. However near $x = 0$ and $x = L$ the complex phases of the different Gaussian functions become important as there are now two functions $\neq 0$ with different phases that we sum over. Here the phase should care for normalization of the total wave function. Furthermore it should make sure that α complies to the general conditions which imply that it is zero at the barriers.

3.3.2 Complex phase of the coherent state α

In this subsection we will show that we can derive from the complex phases of the different peaks that the coherent function we derived satisfies the boundary conditions. Without respect to the complex phase we know that all right-moving and left-moving peaks have different signs. This means that, if we find for every left-moving peak a right-moving peak with the same phase (without respect to the minus sign for the left-moving peaks) and the same absolute value for $x = 0, L$, we can state that the total coherent function α will become zero in the points of discontinuity.

Plugging in $K_j(t)$, the phase of a peak moving to the right with index j becomes:

$$\Theta_j(x,t) = (\phi + 2\pi j)n_0 + \frac{n_0 \pi x}{L} - \frac{\pi^2 \hbar n_0^2 t}{2mL^2} + 2\pi \frac{vt}{L} \frac{(x-\mu_j)^2}{2\sigma(t)^2} \tag{73}$$

with $\mu_j = vt - \phi L/\pi - 2Lj$ and $\sigma(t) = \frac{L}{\sqrt{2\pi|s|}}\sqrt{1 + \left(2\pi \frac{vt}{L}\right)^2}$.

The phase difference between two peaks with j_1 for the right-moving and j_2 for the left-moving (left-moving means that $x \to (-x)$) is:

$$\Delta\theta = 2\pi n_0 (j_1 - j_2) + 2\frac{n_0 \pi x}{L} + 2\pi \frac{vt}{L} \frac{(x-\mu_{j_1})^2 - (x+\mu_{j_2})^2}{2\sigma(t)^2} \tag{74}$$

The first term is always a multiple of 2π, as n_0 is an integer. The same holds for the second part in the points of discontinuity, $x = 0$ and $x = L$. Hence these two terms do not contribution to a phase difference no matter which value we choose for j_1 and j_2. Thus if we want two pairs to have the same phase, we need to find pairs that satisfy the following equation.

$$(x-\mu_{j_1})^2 = (x+\mu_{j_2})^2 \tag{75}$$

The peaks obeying this equation will in addition have equal absolute value. Both sides of the equation represent the numerator of the real exponents of the peaks belonging to j_1 and j_2. The denominator is the same as it is only a function of t. Thus if we find for $x = 0, L$ pairs that obey equation 75, we can state that the boundary conditions are fulfilled.

First let us regard $x = 0$. Plugging in $\mu_{j_{1,2}}$ yields for equation 75:

$$(-vt + \frac{\phi}{\pi}L + 2Lj_1)^2 = (+vt - \frac{\phi}{\pi}L - 2Lj_2)^2 \tag{76}$$

The equation must hold for all $t \in \mathbb{R}$. Therefore the only solution is:

$$j_1 = j_2 \tag{77}$$

Thus every α_j vanishes in 0 and therefore also α.

Now we can use the same procedure for $x = L$. In this case the equation becomes:

$$(L - vt + \frac{\phi}{\pi}L + 2Lj_1)^2 = (L + vt - \frac{\phi}{\pi}L - 2Lj_2)^2 \tag{78}$$

This also has to hold for all $t \in \mathbb{R}$. Therefore we get:

$$L + 2Lj_1 = -L + 2Lj_2 \tag{79}$$

Solving for j_2 yields:

$$j_2 = j_1 + 1 \tag{80}$$

Thus the right-moving peak belonging to j_1 cancels out against the left-moving peak belonging to $j + 2 = j_1 + 1$. Thus here we also have definite pairs of left and right-moving peaks. This means for the coherent function α that it obeys to the boundary conditions and vanishes in $x = 0$ and $x = L$.

3.3.3 Moving Gaussian functions

Without the complex phase we can understand the functions as Gaussian functions with the expectation value μ_j and the uncertainty $\sigma(t)$.

$$\mu_j = vt - \frac{\phi}{\pi}L - 2Lj \tag{81}$$

$$\sigma(t) = \frac{L}{\sqrt{2}\pi|s|}\sqrt{1 + \left(2\pi\frac{vt}{L}\right)^2} \tag{82}$$

Thus finally the coherent wave function can be written as

$$\alpha(x,t) = \sum_{j=-\infty}^{\infty} \alpha_j^{(\mathrm{in})}(x,t) - \sum_{j=-\infty}^{\infty} \alpha_j^{(\mathrm{out})}(x,t) \tag{83}$$

with

$$\alpha_j^{(\mathrm{in})}(x,t) = A_j(t)e^{-\frac{(x-\mu_j)^2}{2\sigma^2} + i\Theta_j(x,t)} \tag{84}$$

and

$$\alpha_j^{(\mathrm{out})}(x,t) = \alpha_j^{(\mathrm{in})}(-x,t) \tag{85}$$

The argument $\Theta_j(x,t)$ of the functions still is given by:

$$\Theta_j(x,t) = (\phi + 2\pi j)n_0 + \frac{n_0\pi x}{L} - \frac{\pi^2\hbar n_0^2 t}{2mL^2} + 2\pi\frac{vt}{L}\frac{(x-\mu_j)^2}{2\sigma(t)^2} \tag{86}$$

In Figure 2 we can see a schematic drawing of the coherent function, which exhibits the incoming and outgoing Gaussian pulses which “reflect” at the walls of the well.

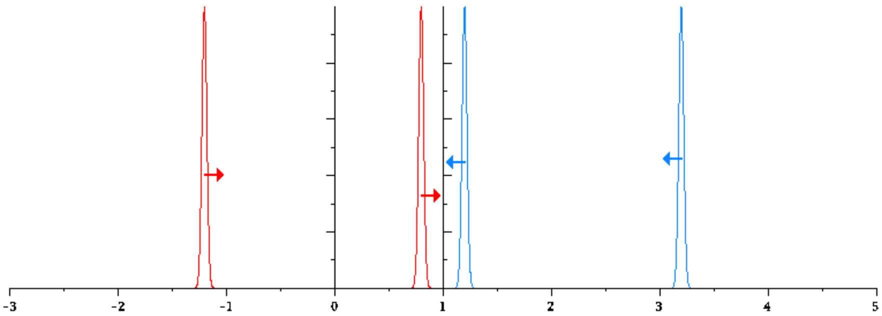

Figure 2: Here we see $\alpha(t)$ in a square well with $L = 1$

3.4 Analysis

Now it is time to put our derived function to the test. As we stated earlier a coherent state has minimal uncertainty in position and momentum.

As it is not easy to determine the uncertainties σ_x and σ_p directly by calculations of $\langle x\rangle$, $\langle x^2\rangle$, $\langle p\rangle$, $\langle p^2\rangle$, we need to analyze α itself.

We can see in equation (81) that our function consist of infinitely many incoming and outgoing Gaussian functions moving at velocity v. All incoming and outgoing peaks have distance $2L$ respectively. This means that there is always one peak on the interval $[0, L]$. As for example the right-moving peak belonging to $j = 0$ arrives at $x = L$, then the left-moving peak belonging to $j = 1$ enters the interval. This can be understood as reflection on the righter barrier of the infinite square well. The same process repeats itself everytime the peak in the box arrives at $x = 0$ or $x = L$. However we do not have any proof that in this process normalization is conserved. However the complex phase makes sure that two peaks always cancel out at the boundaries (see 3.3.2). The most interesting part of the function however is the uncertainty $\sigma(t)$. Assuming that we have a classical limit, we can state with equation (35) that the order of the uncertainty is:

$$\mathcal{O}\left(\sigma(t=0)\right) = L\sqrt{\frac{Js}{\hbar}} \approx L \cdot 10^{-16} \tag{87}$$

Which is very small compared to the length scale of the system. This means that we can speak about a classical system at $t = 0$. However for $t \gg T$ we can neglect the 1 in the square root and the uncertainty becomes:

$$\sigma(t) = \sqrt{2}\pi\frac{vt}{|s|} = \sqrt{2}\pi\frac{2Lt}{T|s|} \approx L\frac{t}{T} \cdot 10^{-16} \tag{88}$$

What we can see in this formula is that also after $2 \cdot 10^6$ reflections at the walls the uncertainty is still only significant in the tenth digit after the point. This still will be difficult to observe, also due to outer influences on the system just as friction or gravity. Therefore we can state that we derived a function that really shows classical behavior when we take the classical limit.

We can also try to have a look at this problem from a different angle. Herefore we will regard a classical system that we give an initial uncertainty in position and momentum. This is also what has happened to the function α we derived in the latter calculation, which has to satisfy Heisenberg's principle.

We will create a state with a free particle with initial values:

$$x = x_0 + \Delta x \tag{89}$$

$$v = v_0 + \Delta v \tag{90}$$

Here we understand $x_0$and v_0 as the expected values and Δx and Δv as a small variation. The equation of motion for a free particle then becomes:

$$x(t) = x_0 + \Delta x + v_0 t + \Delta v t \tag{91}$$

Here we see that last term describing the deviation in the position increases linearly in time. This means that an initial uncertainty in the velocity, will increase the uncertainty in the position during the evolution in time. Therefore it becomes comprehensible that there is a time-dependence in the uncertainty of α. Thus taking this into account we see that the wave function we derived fulfills the requirements for a classical system as good as possible.

However we have to mention that we implicated that the reflection at the barriers has no effect on the uncertainty.

In contrast, for a classical harmonic oscillator a deviation of the initial conditions does not affect the evolution of the state anyhow. With the same initial values the evolution of x can be described with the following equation of motion:

$$x = (x_0 + \Delta x)\cos\omega t + \frac{v_0 + \Delta v}{\omega}\sin\omega \tag{92}$$

with

$$\omega = \sqrt{\frac{k}{m}} \tag{93}$$

which is independent of x and v. What we see is that a variance in position and momentum is possible, however this variance will stay constant for all times. This also applies to the coherent states of a quantum harmonic oscillator (see appendix A).

However the limit $\Delta x, \Delta v \to 0$ will describe the same behavior as the limit $|s| \to \infty$. Hence we can conclude that also for a particle in a box coherent states will become classical for $|s| \to \infty$. Nevertheless we have to mention that this limit also is unphysical as the energy of the system becomes infinite. However for classical energies: $|s| > \mathcal{O}(\sqrt{Js/\hbar})$ this still is an appropriate approximation.

To sum it up, a coherent state in an infinite quantum well has to obey Heisenberg's uncertainty relation. Therefore it always has to have a small amount of uncertainty in position and momentum in the first place. At $t = 0$ this uncertainty is minimal, however with increasing time this uncertainty increases. This can be explainend on the one hand by an evolution of the eigenstates that goes more and more out of phase due to the fact that the energy eigenvalues are not equidistant - $\Delta E_n \sim (n + 1)$ (equation (26)) - as derived in section 2.2.3.

This stands in contrast to the harmonic oscillator that has equidistant energy eigenvalues and whose eigenstate therefore will stay in phase. Hence a coherent state in a harmonic oscillator keeps its minimal uncertainty. On the other hand we derived from the classical equation of motion for a free particle that an initial uncertainty in momentum results in a linear increase of uncertainty in position. Applying this to a particle in a box makes it clear that it will not be possible to create a state that keeps minimal uncertainty during time evolution, unless its uncertainty in momentum is zero.

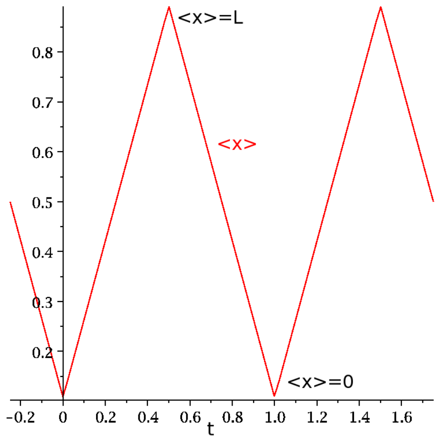

Figure 3: The sawtooth function that shall describe $\langle x \rangle$

4 The classical limit using the Fourier transformation of the sawtooth function

4.1 Preparations

For the calculations in this section we will make use of several formulae that were derived in chapter 3.

In this chapter we are going to analyze the probability function $\langle x \rangle$ and compare it to a sawtooth function f that would describe the movement of a classical particle in a one dimensional box. To obviate complications and to keep calculations simple we will assume that $s \in \mathbb{R}$. This implies that the particle will start at $x = 0$ with velocity $v = \frac{\pi \hbar n_0}{mL}$ (see equation (66)). Hence the sawtooth function we will be using is

$$f(t) = \begin{cases} & \dots \\ -vt & \text{for } -T/2 < t < 0 \\ vt & \text{for } 0 < t < T/2 \\ L - vt & \text{for } T/2 < t < T \\ & \dots \end{cases} \tag{94}$$

We will write this function as a Fourier series:

$$f(t) = \sum_j \beta_j e^{-2\pi i n t/T} \tag{95}$$

with

$$\beta_j = \begin{cases} L/2 & \text{if } j = 0 \\ \frac{L((-1)^j - 1)}{\pi^2 j^2} & \text{if } j \neq 0 \end{cases}$$

and the period $T = \frac{v}{2L}$.

A large s means that the expectation value of the energy of the system is large compared to the ground state. This can be understood as a classical situation (see section 3.1). Hence the purpose is to find an expression for very large $|s| = \mathcal{O}(\sqrt{Js/\hbar})$ which corresponds with a classical system.

From equation (30) we know that the maximum of c_n lies at $n_0 = |s|^2$. As the terms around this maximum have the biggest contribution to the total wave function we will, analog to chapter 3, make use of the substitution:

$$\begin{aligned} n(l) &= n_0 + l \\ m(k) &= n_0 + k \end{aligned} \tag{96}$$

This is what we will be using in the further calculations to to see if the expectation value of the position becomes a sawtooth function.

4.2 $\langle x \rangle$ in the classical limit

The probability function $\langle x \rangle$ is given by

$$\langle x \rangle = \langle \alpha | x | \alpha \rangle = \sum_{n,m} c_n c_m \langle n|x|m \rangle e^{-i(E_m - E_n)t/\hbar} \tag{97}$$

Where the limits of the different parts $c_n c_m$, $\langle n|x|m\rangle$ and $e^{-i(E_m-E_n)t/\hbar}$ will be handled separately in the following three sections.

4.2.1 $\langle n|x|m \rangle$ in the classical limit

$\langle n|x|m\rangle$ can be calculated by integration - see appendix C - which yields:

$$\langle n|x|m \rangle = \begin{cases} L/2 & \text{if } n = m \\ \frac{L}{\pi^2}\left[\frac{(-1)^{n-m}-1}{(n-m)^2} - \frac{(-1)^{n+m}-1}{(n+m)^2}\right] & \text{if } n \neq m \end{cases} \tag{98}$$

Applying equations (96) the term for $n \neq m$ of the expression becomes:

$$\frac{L}{\pi^2}\left[\frac{(-1)^{l-k}-1}{(l-k)^2} - \frac{(-1)^{2n_0+k+l}-1}{(2n_0+k+l)^2}\right] \tag{99}$$

For n_0 large we will neglect the second term, which becomes small compared to the first term due to n_0 in the denominator. If we see $l-k$ as one variable, the resulting expression is the Fourier transform of the sawtooth function:

$$\langle n|x|m \rangle = \begin{cases} L/2 & \text{if } k = l \\ \frac{L}{\pi^2}\frac{(-1)^{l-k}-1}{(l-k)^2} & \text{if } n \neq m \end{cases} = \beta_{l-k} \tag{100}$$

Thus we already derived a first link to the sawtooth function, with $\langle n|x|m\rangle$ which is the corresponding Fourier transform. However we still have two other terms and two sums that have to be transformed to make the sawtooth function complete.

4.2.2 The time evolution term in the classical limit

Here we will again make use of (96) to substitute n and m. Hereby we get the following expression for the exponent of the time evolution term:

$$-i\frac{\pi^2 \hbar t}{2mL^2}(2n_0 k + k^2 - 2n_0 l - l^2) \tag{101}$$

With

$$v = \frac{2L}{T} \tag{102}$$

and equation (66) we arrive at the following expression for the constant factor in the exponent:

$$\frac{\hbar\pi}{2mL^2} = \frac{1}{n_0 T} \tag{103}$$

Substitution yields:

$$-i\pi(2k + \frac{k^2}{n_0} - 2l + \frac{l^2}{n_0})\frac{t}{T} \tag{104}$$

Assuming that $k, l \ll n_0$ we can approximate this with

$$-2\pi i(k-l)\frac{t}{T} \tag{105}$$

If $k - l$ can be seen as one variable, this term is the exponent of the Fourier series. However we still have a double sum and thus we first have to try to derive an expression for the coefficients $c_n c_m$ that makes it possible to separate $k - l$ as index to sum over. In the next section we will see how this is accomplished.

4.2.3 The coefficients $c_n c_m$ in the classical limit

Here we will again make use of the substitution (96). The result is the following equation for the coefficient product:

$$c_n c_m \rightarrow c_l c_k = \frac{s^{2n_0+k+l}}{\sqrt{(n_0+k)!(n_0+l)!}} \tag{106}$$

Let's have a look at the expectation value of the position after the latter calculations:

$$\langle x \rangle = \sum_{k,l} \frac{s^{2n_0+k+l}}{\sqrt{(n_0+k)!(n_0+l)!}} \beta_{l-k} e^{-2\pi i(k-l)t/T} \tag{107}$$

We already mentioned that the $\langle n|x|m\rangle$ part of this equations will become pretty similar to the Fourier series of the sawtooth functions. We can see that β_{k-l} will be the same for all k en l with equal difference. Therefore it seems to be advantageous to make a substitution:

$$\Delta = k - l. \tag{108}$$

However with this substitution we also need to change our understanding of the double sum. In the first place we need to sum over all differences between k and l. Therefore we get a sum over Δ from $-\infty$ to ∞. Here we keep will keep l fixed. Then there will be a second sum over l. With $k = \Delta + l$ the expression for $\langle x \rangle$ becomes:

$$\langle x \rangle = \sum_{l=\infty}^{\infty} \sum_{\Delta=-\infty}^{\infty} \frac{s^{2n_0+\Delta+2l}}{\sqrt{(n_0+\Delta+l)!(n_0+l)!}} \beta_\Delta e^{-2\pi i\Delta t/T} \tag{109}$$

Here we used that β_j is symmetric around 0. We can see that that the expression for the coefficients

$$c_k c_l = \frac{(s^2)^{n_0+l} s^\Delta}{\sqrt{(n_0+\Delta+l)!(n_0+l)!}} \tag{110}$$

becomes rather similar to $|c_n|^2$. Therefore we will try to "extract" the Δ from the denominator. Rewriting the factorial yields:

$$\begin{aligned}(n_0+\Delta+l)!(n_0+l)! &= (n_0+l)!\frac{(n_0+\Delta+l)!}{(n_0+l)!}(n_0+l)! \\ &= ((n_0+l)!)^2 \frac{(n_0+\Delta+l)!}{(n_0+l)!}\end{aligned} \tag{111}$$

If we assume that a variation in l has no great effect on the variation on n_0+l - which is comprehensible if we suppose that terms far away from the maximum in c_n will not contribute to the probability function - we can approximate the fraction in (111) with

$$\frac{(n_0+\Delta+l)!}{(n_0+l)!} \approx n_0^\Delta = |s|^{2\Delta} \tag{112}$$

Thus we can write

$$c_k c_l \approx \frac{s^{2(n_0+l)}}{(n_0+l)!} = |c_{n_0+l}|^2 \tag{113}$$

and as a result the double sum can be divided into two separate sums:

$$\langle x \rangle \approx \sum_l |c_{n_0+l}|^2 \sum_\Delta \beta_\Delta e^{-2\pi i \Delta t/T} \tag{114}$$

The first sum is 1 due to normalization - see equation 8 - and the second sum is the Fourier Series of the sawtooth function. So we can state that

$$\lim_{|s|\to\infty} \langle x \rangle = \sum_\Delta \beta_\Delta e^{-2\pi i \Delta t/T} = f(x) \tag{115}$$

Thus we can state that the expectation value of the position for a coherent function in an infinite square well will become a sawtooth function in the classical limit.

4.3 Analysis

The result is exactly the equation of motion which we would expect for a classical particle in a box. Therefore we can conclude that in the classical limit a coherent state leads to quasiclassical behavior. However this is just the expectation value. We cannot conclude much about the uncertainty in the position for the particle for we did not calculate $\langle x^2 \rangle$. Doing this in addition would indeed be interesting, however this will not be a subject to this article.

Though what we can conclude is that at $x = 0$ and $x = L$ the uncertainty must go to zero in the classical limit. Otherwise it would not be possible for $\langle x \rangle$ to "reach" the boundaries. For an infinite square well it is not possible for the particle to get over the boundaries. Therefore the probability for $x > L$ and $x < 0$ is zero. Thus if the expectation value is $x = 0$ or $x = L$ and if there is an uncertainty larger than zero there has to be a chance for the particle to be at positions to the left and to the right of a boundary. This contradicts with the fact that there is no chance of finding the particle behind a boundary. Therefore we can conclude that the uncertainty in the position is zero when the particle hits a boundary. However at these points the particle reflects at the boundary. Since the boundaries are infinite there is a discontinuity in the velocity of the particle at the points $x = 0$ and $x = L$. We cannot determine whether the particle is moving right or left. Thus the uncertainty in momentum is infinite.

In the the latter calculation we have assumed that s is real. However generally this is not true. Though this will not be a subject of this article, it might be interesting to do the same calculations on the assumption that s is complex. What we will expect then is a phase shift in the Fourier series, so that the starting position of the particle will be dependent on the complex phase of s just like in section 3.

5 Conclusion

Let us resume the results of the two preceding approaches: The direct calculation of the coherent state α resulted in two sets of equidistant Gaussian functions moving with uniform velocity v in opposed directions. The uncertainty is inversely proportional to $|s|$ and becomes negligible in the classical limit and for $t \ll T \cdot 10^6$. It increases under time evolution. From a quantum mechanical point of view this means that the eigenstates building up the coherent function will run more and more out of phase, hereby the whole function will become more incoherent with increasing time. Consequently there is no minimal uncertainty in position and momentum under time evolution just as anticipated in section 2.2.3. This stands in a contrast to coherent states in a harmonic oscillator where minimal uncertainty is preserved under time evolution. However with respect to the classical equations of motion we could see that also the position of a classical particle in a box will become less certain if there is an initial uncertainty in the momentum. This supports the result of chapter 3. The second approach showed us that also the expectation value of the position becomes classical in the limit. In addition we could conclude that the uncertainty of the position becomes zero at the boundaries. However at these points the momentum of the particle is entirely undetermined. Therefore it is not possible speak of minimal uncertainty in position and momentum. Though we are able to conclude, that if $\langle x \rangle$ converges to a sawtooth function its wavefunction will not be able to spread out under time evolution. Otherwise $\langle x \rangle$ would not be able to reach the boundaries anymore where minimal uncertainty in the position is crucial. However we have to mention that this may result from the limit we have taken. For example the quadratic terms in the time evolution terms of $\langle x \rangle$ may have certain influence on the phase differences of the different eigenstates which could lead to a dispersing wavefunction.

We see that there are certain contradictions between the results of the two approaches. To find the causes we can investigate the different approximations. Maybe some of them where too vigorous and disturbed the results.

All in all we can conclude that coherent states in an infinite square well will lead to classical behavior under application of the classical limit. However they do not preserve minimal uncertainty as the coherent states of a harmonic oscillator. To create such states in a quantum box we would need to search for functions that will preserve phase coherence of the eigenstates under time evolution.

A Coherent states of the harmonic oscillator

For the harmonic oscillator we can define the following Hamiltonian:

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + 1) \tag{116}$$

Whereas $\hat{a}^\dagger$ and $\hat{a}$ are the raising and lowering (ladder) operators which are given by

$$\begin{aligned}\hat{a} &= \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} + i\hat{p}) \\ \hat{a}^\dagger &= \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{x} - i\hat{p})\end{aligned} \tag{117}$$

So that under substitution we will get the familiar form of the Hamiltonian, the sum of kinetic and potential energy:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{118}$$

The coherent states are the eigenfunctions of the lowering operator and satisfy equation (15). To find the uncertainties in position and momentum we will first calculate $\langle\hat{x}\rangle$, $\langle\hat{x}^2\rangle$, $\langle\hat{p}\rangle$ and $\langle\hat{p}^2\rangle$. Herefore we solve equations 117 for $\hat{x}$ and $\hat{p}$:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a});\ \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}^\dagger - \hat{a}) \tag{119}$$

Now we can substitute $\hat{x}$ and $\hat{p}$ with the lowering and raising operator:

$$\begin{aligned}\langle\hat{x}\rangle =& \sqrt{\frac{\hbar}{2m\omega}}\langle\alpha|\hat{a}^\dagger + \hat{a}|\alpha\rangle \\ =& \sqrt{\frac{\hbar}{2m\omega}}\left(\langle\alpha|\hat{a}^\dagger|\alpha\rangle + \langle\alpha|\hat{a}|\alpha\rangle\right) \\ =& \sqrt{\frac{\hbar}{2m\omega}}\left(s^* + s\right)\end{aligned}$$

$$\begin{aligned}\langle\hat{x}^2\rangle =& \frac{\hbar}{2m\omega}\langle\alpha|\hat{a}^\dagger\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}\hat{a}|\alpha\rangle \\ =& \frac{\hbar}{2m\omega}\langle\alpha|(s^*)^2 + s^*s + 1 + s^*s + s^2|\alpha\rangle \\ =& \frac{\hbar}{2m\omega}\left(s^{*2} + 2ss^* + s^2 + 1\right)\end{aligned}$$

$$\begin{aligned}\langle\hat{p}\rangle =&i\sqrt{\frac{\hbar m\omega}{2}}\langle\alpha|\hat{a}^\dagger-\hat{a}|\alpha\rangle\\=&i\sqrt{\frac{\hbar m\omega}{2}}\langle\alpha|s^*-s|\alpha\rangle\\=&i\sqrt{\frac{\hbar m\omega}{2}}\left(s^*-s\right)\end{aligned}$$

$$\begin{aligned}\langle\hat{p}^2\rangle =&-\frac{\hbar m\omega}{2}\langle\alpha|\hat{a}^\dagger\hat{a}^\dagger-\hat{a}^\dagger\hat{a}-\hat{a}\hat{a}^\dagger+\hat{a}\hat{a}|\alpha\rangle\\=&-\frac{\hbar m\omega}{2}\langle\alpha|s^{*2}-s^*s-1-s^*s+s^2|\alpha\rangle\\=&-\frac{\hbar m\omega}{2}\left(s^{*2}-2ss^*+s^2-1\right)\end{aligned}$$

Here we used that $[\hat{a},\hat{a}^\dagger]=1$ and equation (15). Now the uncertainties in position and momentum are easily calculated:

$$\begin{aligned}\sigma_x &= \sqrt{\langle\hat{x}^2\rangle-\langle\hat{x}\rangle^2}\\&=\sqrt{\frac{\hbar}{2m\omega}\left(s^{*2}+2ss^*+s^2+1-(s^*+s)^2\right)}\\&=\sqrt{\frac{\hbar}{2m\omega}}\end{aligned}$$

$$\begin{aligned}\sigma_p &= \sqrt{\langle\hat{p}^2\rangle-\langle\hat{p}\rangle^2}\\&=\sqrt{\frac{\hbar m\omega}{2}\left[-\left(s^{*2}-2ss^*+s^2-1\right)-i^2(s^*-s)^2\right)}\\&=\sqrt{\frac{\hbar m\omega}{2}}\end{aligned}$$

Thus the uncertainty product is minimal:

$$\sigma_p\sigma_x=\frac{\hbar}{2} \tag{120}$$

Now we will check if a coherent function of the harmonic oscillator stays coherent under time evolution.

From chapter 2.2 we know that the expansion coefficients of this function have to comply with equation (20). Thus we can write for the coherent function $|\alpha\rangle$ with timedependence:

$$|\alpha\rangle=\sum_n c_n|n\rangle e^{-iE_nt/\hbar} \tag{121}$$

Now we let the lowering operator work on $|\alpha\rangle$:

$$\begin{aligned}\hat{a}|\alpha\rangle &= \sum_{n=0}^{\infty} c_n\sqrt{n}|n-1\rangle e^{-iE_nt/\hbar} \\ &= \sum_{n=0}^{\infty} \frac{s}{\sqrt{n}} c_{n-1}\sqrt{n}|n-1\rangle e^{-i(E_{n-1}+\hbar\omega)t/\hbar} \\ &= se^{-i\omega t}\sum_{n=0}^{\infty} c_{n-1}|n-1\rangle e^{iE_{n-1}t/\hbar}\end{aligned}$$

As $\hat{a}|0\rangle = 0|0\rangle$ we can start the sum at $n = 1$ and it becomes the expression for the coherent function. Thus the new time-dependent eigenstate equation is:

$$\hat{a}|\alpha\rangle = se^{-i\omega t}|\alpha\rangle \tag{122}$$

Hence $|\alpha\rangle$ remains an eigenstate of $\hat{a}$ with the time-dependent eigenvalue

$$s(t) = se^{-i\omega t} \tag{123}$$

Consequently the coherent state of the harmonic oscillator stays coherent and continues to minimize the uncertainty product.

The expectation value of the position becomes with equation (123):

$$\langle\hat{x}\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,(s^* + s) \tag{124}$$

$$= \sqrt{\frac{\hbar}{2m\omega}}2\Re(se^{-i\omega t}) \tag{125}$$

$$= \sqrt{\frac{\hbar}{2m\omega}}2|s|\cos(\omega t - \arg(s)) \tag{126}$$

Now we equal the expected eigenenergy of the state with the classical energy of a an oscillator.

$$E_{n_0} \approx \hbar\omega|s|^2 \approx \frac{1}{2}mx_0^2\omega^2 \tag{127}$$

With x_0 the amplitude of the oscillation. Solving the above equation for x_0 yields the constant factor in (126). Thus the expectation value of the position becomes:

$$\langle\hat{x}\rangle = x_0\cos(\omega t - \arg(s)) \tag{128}$$

Which is the classical equation of motion for a harmonic oscillator.

B Fourier transformation of $f(x)$

In this section we will derive the Fourier series of the sawtooth function that has been used to show that a classical limit of a coherent state in an infinite square well results classical behavior. First we need to define the connection between a function and its Fourier transformation. In this article we will use the following definition:

$$f(t) = \sum_{j=-\infty}^{\infty} \beta_j e^{-2\pi i j t/T} \tag{129}$$

$$\beta_j = \frac{1}{T}\int_{t_0}^{t_0+T} f(t) e^{2\pi i j t/T} \tag{130}$$

Here f(t) will be the sawtooth function that corresponds with the position of a classical particle. We write:

$$f(t) = \begin{cases} & ... \\ -vt & \text{for } -T/2 < t < 0 \\ vt & \text{for } 0 < t < T/2 \\ L - vt & \text{for } T/2 < t < T \\ & ... \end{cases} \tag{131}$$

To calculate the Fourier series β_j we have to solve (130). First we calculate β_0. With $t_0 = -T/2$ we get:

$$\beta_0 = \frac{1}{T}\int_{-T/2}^{T/2} dt\ f(t) e^0 \tag{132}$$

$$= \frac{v}{T} 2 \int_{0}^{T/2} dt\ t \tag{133}$$

$$= \frac{v}{T}\frac{T^2}{4} = \frac{vT}{4} = \frac{L}{2} \tag{134}$$

For $j \neq 0$ however we have to use partial integration to solve β_j:

$$
\begin{aligned}
\beta_j =& \frac{1}{T}\int_{-T/2}^{T/2} dt \;\; f(t) e^{2\pi i j t/T} \\
=& \frac{v}{T}\left[\int_{-T/2}^{0} dt \;\; (-t) e^{2\pi i j t/T} + \int_{0}^{T/2} dt \;\; t e^{2\pi i j t/T}\right] \\
=& \frac{v}{T}\left[-\left[t\frac{T}{2\pi i j} e^{2\pi i j t/T}\right]_{-T/2}^{0} + \int_{-T/2}^{0} dt \;\; \frac{T}{2\pi i j} e^{2\pi i j t/T}\right. \\
& \left. + \left[t\frac{T}{2\pi i j} e^{2\pi i j t/T}\right]_{0}^{T/2} - \int_{0}^{T/2} dt \;\; \frac{T}{2\pi i j} e^{2\pi i j t/T}\right] \\
=& \frac{v}{T}\left[-\left[0 + \frac{T^2}{4\pi i j} e^{-\pi i j}\right] + \left[\left(\frac{T}{2\pi i j}\right)^2 e^{2\pi i j t/T}\right]_{-T/2}^{0}\right. \\
& \left. + \left[\frac{T^2}{4\pi i j} e^{\pi i j} - 0\right] - \left[\left(\frac{T}{2\pi i j}\right)^2 e^{2\pi i j t/T}\right]_{0}^{T/2}\right] \\
=& \frac{v}{T}\left[\frac{T^2}{4\pi i j}\left((-1)^j - (-1)^j\right) + \left[\left(\frac{T}{2\pi i j}\right)^2 \left(1 - e^{\pi i j}\right)\right]\right. \\
& \left. - \left[\left(\frac{T}{2\pi i j}\right)^2 \left(e^{\pi i j} - 1\right)\right]\right] \\
=& \frac{v}{T}\left(\frac{T}{2\pi i j}\right)^2 \left[0 + 1 - (-1)^j - (-1)^j + 1\right] \\
=& \frac{vT}{2\pi^2 j^2}((-1)^j - 1)
\end{aligned}
$$

with $L = \frac{vT}{2}$ this results in:

$$
\beta_j = \frac{L((-1)^j - 1)}{\pi^2 j^2} \tag{135}
$$

C Calculation of $\langle n|x|m\rangle$

In this section we will derive an expression for $\langle n|x|m\rangle$. First let's have a look at the special case $n = m$:

$$
\begin{aligned}
\langle n|x|n\rangle =& \frac{2}{L}\int_0^L dx x \sin^2\left(\frac{n\pi x}{L}\right) \\
=& \frac{1}{L}\int_0^L dx (x - x\cos\left(\frac{2n\pi x}{L}\right) \\
=& \frac{1}{L}\left[\frac{1}{2}L^2 - \left[x\left(\frac{L}{2n\pi}\right)\sin\left(\frac{2n\pi x}{L}\right)\right]_0^L + \int_0^L dx \left(\frac{L}{2n\pi}\right)\sin\left(\frac{2n\pi x}{L}\right)\right]
\end{aligned}
$$

Here the second term is zero because $\sin n\pi = 0 \forall n \in \mathbb{N}$. In addition the last term has no contribution either as integration yields a term containing $\cos 2n\pi - 1 = 0 \forall n \in \mathbb{N}$. Thus:

$$\langle n|x|n\rangle = \frac{1}{2}L \tag{136}$$

For $n \neq m$ we use the trigonometric identity

$$\sin\alpha\sin\beta = \frac{1}{2}\left(\cos(\alpha-\beta) - \cos(\alpha+\beta)\right) \tag{137}$$

Then we solve with integration by parts:

$$\begin{aligned}
\langle n|x|m\rangle =& \frac{2}{L}\int_0^L dx \;\; x\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right) \\
=& \frac{1}{L}\int_0^L dx \;\; \left(x\cos\frac{(n-m)\pi x}{L} \;\; - \cos\frac{(n+m)\pi x}{L}\right) \\
=& \frac{1}{L}\left[\left[x\left(\frac{L}{(n-m)\pi}\sin\frac{(n-m)\pi x}{L} \;\; - \frac{L}{(n+m)\pi}\sin\frac{(n+m)\pi x}{L}\right)\right]_0^L \right. \\
& \left. - \int_0^L dx \;\; \left(\frac{L}{(n-m)\pi}\sin\frac{(n-m)\pi x}{L} \;\; - \frac{L}{(n+m)\pi}\sin\frac{(n+m)\pi x}{L}\right)\right]
\end{aligned}$$

The first term is zero because $\sin n\pi = 0 \forall n \in \mathbb{N}$. Integrating the second part and using $\cos n\pi = (-1)^n \forall n \in \mathbb{N}$ we get:

$$\langle n|x|m\rangle = \frac{l}{\pi^2}\left[\frac{(-1)^{n-m}-1}{(n-m)^2} - \frac{(-1)^{n+m}-1}{(n+m)^2}\right] \tag{138}$$

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