

# Cavity QED with cold particles

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### **Abstract**

We motivate and derive a theoretical model arranging atoms in a lattice to simulate a solid. For that, we'll make use of atom-light field interaction which is enhanced in a cavity. After deriving the Hamiltonians for our systems, we'll discuss some of their properties. We'll then conduct simulations in the language Julia with the framework QuantumOptics.jl to see if we can observe the properties we expect our systems to have.

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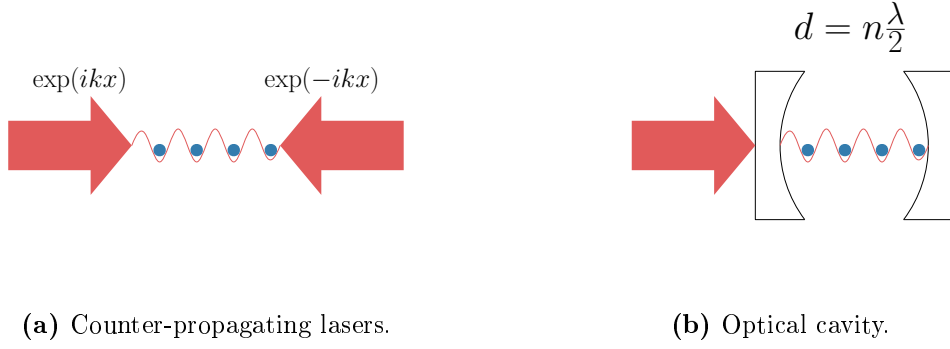
# 1 Introduction

The study of solid-state objects is of great interest for us, especially since some phenomena occurring in solids have a lot of commercial potential. There are some difficulties, however. It can be very challenging to look into a solid. Certain phenomena might be happening very fast (e.g. on a nanosecond scale), the lattice spacing might be very small (e.g. only several angstroms apart) and in every naturally occurring solid there are structural defects and lattice vibrations. All these things can obfuscate the basic workings of certain phenomena. On top of all that, we can't change a naturally occurring solid which is probably the biggest inconvenience. A way to circumvent all these problems is to just make a crystal ourselves, a crystal in which certain phenomena are happening much slower (e.g. on a second scale), in which there's a bigger lattice spacing (e.g. on a micrometer scale) and that is free of defects. That crystal will be fully controllable by us and we can change its structure as we wish.

In this thesis, we'll ask ourselves the question how to make atoms self-organize to create an artificial solid. For that, we'll establish a theoretical model in which we arrange atoms in a lattice. We'll obtain two configurations with two Hamiltonians whose properties we'll discuss. Simulations in the language Julia with the framework QuantumOptics.jl will show us if we're able to observe the properties that we expect.

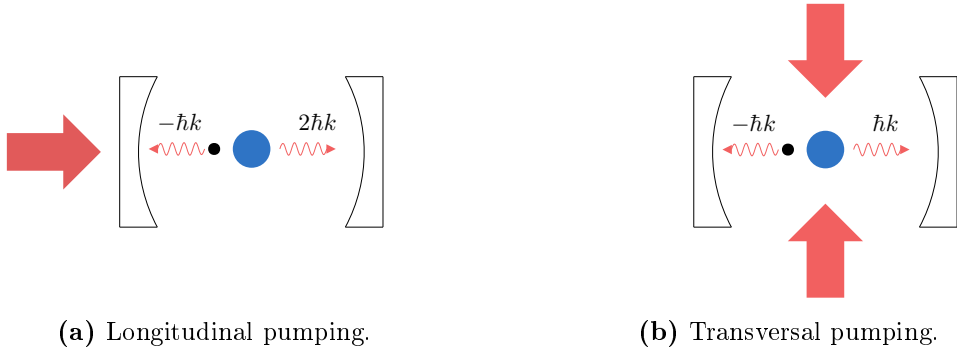
## 2 Explanation of the model

What we want to achieve is to arrange atoms in a lattice to simulate a solid. We need to somehow hold them in place. For that, we'll use laser light. Consider the setup depicted in Figure 1a. There are two lasers, each with the same frequency. If we set their direction on the same axis, but counter propagating with contributions  $\propto \exp(ikx)$  and  $\propto \exp(-ikx)$ , a cosine pattern or standing wave of the intensity will form. In between, we put our atoms. There's a special trick now. We set the frequency of the laser  $\omega_l$  way below the excitation frequency of the atoms  $\omega_a$  (this is commonly called "red-detuning"). That will induce dipoles in the atoms and the dipoles will interact with the light field. Because of the dipole-light field interaction, there's now a potential for the atoms which is what we needed. The atoms will now sort of "fall" into the lowest points of the potential to minimize their energy. The light field intensity has a cosine pattern, thus the same will be the case for the potential ( $V \propto -I$ ). Now we have an array of equally spaced atoms, already what we could call an artificial solid. To enhance atom-light field interaction, we'll take our setup one step further and introduce a cavity, as depicted in Figure 1b. There are two mirrors. The one on the left is partially transmissive to let the laser light in. We set the distance between the two mirrors to  $d = n\lambda/2$  so that the light field will be amplified inside the cavity.



**Figure 1:** Two counter-propagating lasers create a cosine-potential. In between, we put our atoms. Red-detuning the lasers will induce dipoles in the atoms which interact with the light field, creating a potential for the atoms. As the atoms always strive to minimize their energy, they will position themselves at the "valleys" of the potential. We'll take that approach even further and put the atoms in a cavity. That way atom-light field interaction will be enhanced.

There are different ways to get a light field inside the cavity. Figure 2a depicts what we've discussed so far. There we shoot a laser parallel to the cavity axis into the cavity (longitudinal pump). Even if there are no atoms inside, there's still a light field. That is not the case if we pump transversally, as described in [1] and shown in Figure 2b. For transversal pump, if there are no atoms inside the cavity, no light field will exist along the cavity axis. To create a light field, here we rely on the atoms scattering the photons into the cavity, i.e. the atoms effectively create their own trapping potential. Pumping transversally, a couple interesting phenomena emerge which do not happen for the longitudinal pump. We will discuss those properties later. Now to the derivation of the Hamiltonians for those two systems.



**Figure 2:** Longitudinally and transversally pumped cavities. For longitudinal pumping, even if there are no atoms inside the cavity, there's still a light field. That is not the case for transversal pumping. There the light field along the cavity axis is created by the atoms scattering incoming photons, i.e. the atoms are effectively creating their own trapping potential.

### 3 Derivation of the Hamiltonians

For those wishing to refresh their knowledge in quantum mechanics, the introductory chapters of Fox's quantum optics book will be of great help [2] (it's a great quantum optics book in general). In this section we'll derive the Hamiltonians being used for the simulation: One Hamiltonian for longitudinal pumping and one for transversal pumping. We'll start with the Jaynes-Cummings Hamiltonian which describes the interaction of a two-level atom with a single mode of a cavity-field. We'll then modify the Hamiltonian according to our needs step by step. We'll tackle the crucial details and reference parts of the derivation which are not presented here.

#### 3.1 The Jaynes-Cummings Hamiltonian

The Jaynes-Cummings model describes the interaction of a two-level atom with a single mode of a cavity field. The first appearance of the model was in [3]. Since we're dealing with both an atom and a light field at the same time, we have a composite system, i.e.

$$\psi_{\text{total}} = \psi_{\text{light}} \otimes \psi_{\text{atom}}. \quad (1)$$

The fact that we have two levels motivates a two-dimensional basis for the atom:

$$|g\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |e\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (2)$$

where  $|g\rangle$  is the ground state and  $|e\rangle$  is the excited state. Both states respond to the operators

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad (3)$$

where  $\sigma^+$  is the raising operator and  $\sigma^-$  is the lowering operator. They have the properties

$$\sigma^+|g\rangle = |e\rangle, \quad \sigma^-|e\rangle = |g\rangle. \quad (4)$$

The wave function for the atoms depends on the position, while this is not the case for the light field. Instead we will use photon number states or Fock states. A photon number state  $|n\rangle$  thus represents a monochromatic quantized field containing  $n$  atoms. The ground state  $|0\rangle$  corresponds to 0 photons. The creation and annihilation operators  $a^\dagger$  and  $a$  correspond to creating and annihilating a photon. We'll restrict ourselves to one dimension and start with an atom (or a Bose-Einstein condensate) in an external potential:

$$H_0 = \frac{p^2}{2m} + V_{\text{ext}}(x). \quad (5)$$

Now we place that atom in a cavity and it will interact with the cavity mode, creating more terms in our Hamiltonian that we have to consider. First, there's the energy of the field:

$$H_{\text{field}} = -\hbar\omega_c a^\dagger a, \quad (6)$$

where  $\omega_c$  is the resonance frequency of the cavity and  $a^\dagger$  and  $a$  are the creation and annihilation operators. Next, we'll add a term describing the atomic transitions:

$$H_{\text{transition}} = -\hbar\omega_a \sigma_z, \quad (7)$$

where  $\omega_a$  is the resonance frequency of the atom and  $\sigma_z$  is the Pauli  $z$ -matrix which is defined as  $\sigma_z = 1/2(|e\rangle\langle e| + |g\rangle\langle g|)$  or

$$\sigma_z = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}. \quad (8)$$

The Hamiltonian  $H_{\text{transition}}$  describes the atom being in the ground state or excited state, the transition energy is  $\hbar\omega_a$ . The atom-field interaction we describe with following term:

$$H_{\text{interaction}} = \hbar g_0 \cos(kx)(\sigma^+ a + \sigma^- a^\dagger), \quad (9)$$

where  $g_0$  is the coupling strength. Finally, we'll add the term describing the pumping:

$$H_{\text{pump}} = \hbar\eta(ae^{i\omega_l t} + a^\dagger e^{-i\omega_l t}), \quad (10)$$

where  $\eta$  is the pumping strength and  $\omega_l$  is the laser frequency. We now have the full Jaynes-Cummings Hamiltonian which is the sum of all terms above:

$$H_{\text{JC}} = \underbrace{p^2/2m}_{\text{atom}} + \underbrace{V_{\text{ext}}(x)}_{\text{external potential}} - \underbrace{\hbar\omega_a \sigma_z}_{\text{atomic transitions}} - \underbrace{\hbar\omega_c a^\dagger a}_{\text{field}} + \underbrace{\hbar\eta(ae^{i\omega_l t} + a^\dagger e^{-i\omega_l t})}_{\text{pumping}} + \underbrace{\hbar g_0 \cos(kx)(\sigma^+ a + \sigma^- a^\dagger)}_{\text{field-atom interaction}}. \quad (11)$$

A more detailed derivation of the Jaynes-Cummings Hamiltonian (starting from Maxwell's equations and quantizing the cavity mode) can be found at [4]. In order to get rid of the explicit time-dependence, we transform the Hamiltonian to a frame rotating with  $\omega_l$ . The Hamiltonian now reads:

$$H_{\text{JC}} = \frac{p^2}{2m} + V_{\text{ext}}(x) + \hbar\Delta_a \sigma_z - \hbar\Delta_c a^\dagger a + \hbar\eta(a + a^\dagger) + \hbar g_0 \cos(kx)(\sigma^+ a + \sigma^- a^\dagger), \quad (12)$$

where  $\Delta_a = \omega_l - \omega_a$  and  $\Delta_c = \omega_l - \omega_c$ .

### 3.2 Detuning

The derivation for the Hamiltonians for the following sections is taken from [5]. Now we derive heuristically a modified Hamiltonian. Going to the Heisenberg picture, we get:

$$\dot{a} = \frac{i}{\hbar}[H, a] = i\Delta_c a - i\eta - ig_0 \cos(kx)\sigma^-. \quad (13)$$

Obviously, the kinetic energy and potential term vanish under the commutator. For the other terms:

$$a^\dagger a = N, \quad [N, a] = -a, \quad (14)$$

$$(a + a^\dagger)a - a(a + a^\dagger) = aa + a^\dagger a - aa - aa^\dagger = 1 \quad (15)$$

$$\text{because we know: } aa^\dagger = a^\dagger a + 1,$$

$$[\sigma^+ a + \sigma^- a^\dagger, a] = \sigma^+ \underbrace{[a, a]}_0 + \sigma^- \underbrace{[a^\dagger, a]}_1 = \sigma^-. \quad (16)$$

The creation and annihilation operators ( $a^\dagger$  and  $a$ ) and the raising and lowering operators ( $\sigma^+$  and  $\sigma^-$ ) live in different Hilbert spaces and thus don't influence each other. A good reference for the commutator relation is [6]. The time-derivative for the raising operator reads:

$$\dot{\sigma}^+ = \frac{i}{\hbar}[H, \sigma^+] = \underbrace{-i\Delta_a \sigma^+}_{(*)} + \underbrace{ig_0 \cos(kx)a^\dagger}_{(**)}. \quad (17)$$

For (\*), we'll look at the matrix representation of the operators:

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}. \quad (18)$$

We calculate the commutator relation  $[\sigma_z, \sigma^+]$  explicitly:

$$\begin{aligned} [\sigma_z, \sigma^+] &= \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix} = \\ &= \begin{pmatrix} 0 & 1/2 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & -1/2 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \sigma^+. \end{aligned} \quad (19)$$

For (\*\*), we'll calculate  $[\sigma^-, \sigma^+]$ :

$$\begin{aligned} [\sigma^-, \sigma^+] &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \\ &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = -2\sigma_z \approx 1. \end{aligned} \quad (20)$$

In our case, the pumping laser is far detuned from the atomic resonance frequency, i.e.  $\omega_l \ll \omega_a$ . The atom thus only stays in the ground state and we approximate  $\sigma_z \approx -1/2$ . Since we're not interested in fast dynamics, we set  $\dot{\sigma}^+ = 0$ . We get:

$$\sigma^+ = \frac{g_0}{\Delta_a} \cos(kx) a^\dagger, \quad \sigma^- = \frac{g_0}{\Delta_a} \cos(kx) a. \quad (21)$$

Putting the above relation in equation 13, we get:

$$\dot{a} = -i\Delta_c a + \frac{ig_0}{\Delta_a} \cos(kx) a - i\eta. \quad (22)$$

We can thus make a guess of the effective Hamiltonian:

$$H_{\text{long}} = \frac{p^2}{2m} + V_{\text{ext}}(x) - \hbar\Delta_c a^\dagger a + \hbar\eta(a + a^\dagger) + \hbar U_0 \cos(kx)^2 a^\dagger a, \quad (23)$$

where we set  $U_0 := g_0^2/\Delta_a$ . Note that because  $H_{\text{long}} \propto \cos(kx)^2$ , the Hamiltonian is  $\lambda/2$ -periodic. Later in the simulation program, we want to make sure all quantities are expressed in terms of the recoil energy  $E_r = \hbar\omega_r$ , where  $\omega_r = \hbar k^2/2m$  is the recoil frequency. Therefore we factor our  $E_r$  to see what we have to type into the program:

$$H_{\text{long}} = \hbar\omega_r \left( \frac{1}{\hbar^2 k^2} p^2 + \frac{1}{\hbar\omega_r} V_{\text{ext}}(x) - \frac{1}{\omega_r} \Delta_c a^\dagger a + \frac{1}{\omega_r} \eta(a + a^\dagger) + \frac{1}{\hbar\omega_r} U_0 \cos(kx)^2 a^\dagger a \right). \quad (24)$$

In the simulation program, we will set  $\hbar = 1$  and multiply each quantity by the preceding factors.

### 3.3 Transversal Pump

Now we'll tackle the transversal pump. Here the cavity mode will only be populated by photons which were scattered off the atoms. The Hamiltonian now reads:

$$H_{\text{trans}} = \frac{p^2}{2m} + V_{\text{ext}}(x) - \hbar\Delta_c a^\dagger a + \hbar\eta \cos(kx) \cos(kz)(a + a^\dagger) + \hbar \frac{\Omega^2}{\Delta_a} \cos(kz)^2 + \hbar U_0 \cos(kx)^2 a^\dagger a, \quad (25)$$

where  $\Omega$  is the Rabi frequency. Here we only consider one dimension, so we set  $z = 0$ :

$$H_{\text{transv}} = \frac{p^2}{2m} + V_{\text{ext}}(x) - \hbar\Delta_c a^\dagger a + \hbar\eta \cos(kx)(a + a^\dagger) + \hbar U_0 \cos(kx)^2 a^\dagger a. \quad (26)$$



Note that because  $H_{\text{trans}} \propto \cos(kx)$ , the Hamiltonian is  $\lambda$ -periodic. The only difference now to the longitudinal pump Hamiltonian is the spatial dependence in the pump term.

## 4 Properties of the system

We'll now discuss some properties that the longitudinally and transversally pumped cavities have and later tackle some further details only concerning the transversally pumped cavity. There is a fundamental difference how atoms scatter light in the longitudinally pumped cavity and in the transversally pumped cavity. For the longitudinal pump, if a photon with momentum  $\hbar k$  in  $x$ -direction bumps into an atom, it will recoil backward, having now a momentum  $-\hbar k$ . Conservation of momentum thus requires the atom to have now a momentum of  $2\hbar k$ . For the transversal pump, when a photon is incident perpendicularly to the cavity axis, the total momentum in the  $x$ -direction will be 0. If an atom scatters now the photon along the cavity axis, it will now have a momentum of  $\hbar k$  and the photon  $-\hbar k$ . The total momentum along the  $x$ -direction will still be 0. We see that the fundamental difference between longitudinal and transversal pump is the momenta the atoms are able to acquire. In the longitudinal case, there will only be momenta of  $2n\hbar k$ , where  $n \in \mathbb{N}$ , whereas for the transversal pump there are momenta of  $\hbar k$ . To illustrate the discrete momenta, take a look at the wave function representing the atoms inside the cavity:

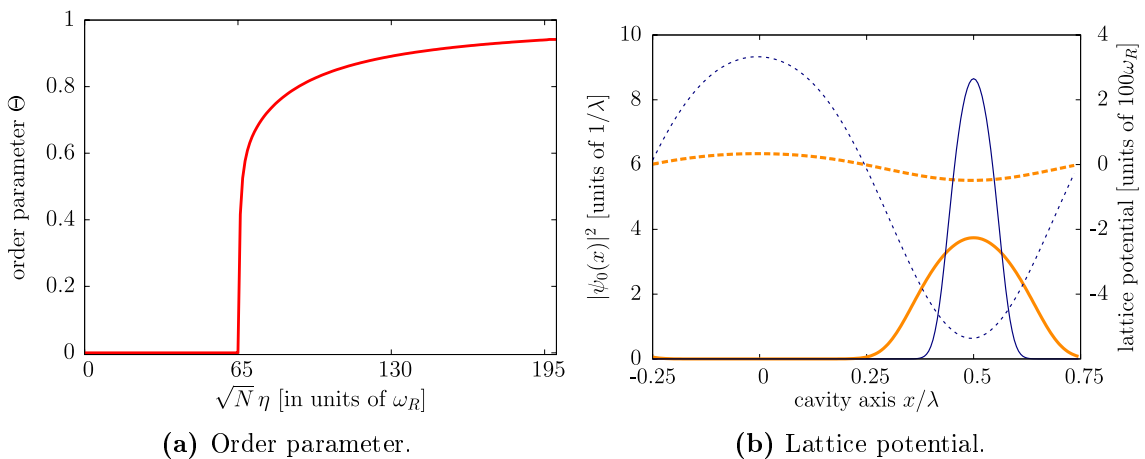
$$\psi(x) = \frac{1}{N} \sum_l c_l \exp(likx) = \frac{1}{N} \left( c_0 + c_{\pm 1} \exp(ikx) + c_{\pm 2} \exp(2ikx) + \dots \right). \quad (27)$$

The variable  $N$  is a normalizing constant. As previously mentioned, an atom inside the cavity cannot have any arbitrary momentum, but only multiples of  $\hbar k$  due to the way momentum is acquired. If we plot the wave function as a whole, we don't see the discreteness of the momenta. However, if we perform a Fourier transform, we can access the  $c_l$ 's. For longitudinal pump, we thus only expect momenta of 0,  $2\hbar k$ ,  $4\hbar k$ ,  $\dots$  corresponding to  $c_0$ ,  $c_{\pm 2}$ ,  $c_{\pm 4}$  and so on. For transversal pump we expect momenta of 0,  $\hbar k$ ,  $2\hbar k$ ,  $3\hbar k$ ,  $\dots$  corresponding to  $c_0$ ,  $c_{\pm 1}$ ,  $c_{\pm 2}$ ,  $c_{\pm 3}$  and so on. In Table 4 there are the  $c_l$ 's with the components of the wave function.

$c_l$	wave number	momentum
$c_0$	0	0
$c_{\pm 1}$	$k \rightarrow \exp(ikx)$	$\hbar k$
$c_{\pm 2}$	$2k \rightarrow \exp(2ikx)$	$2\hbar k$
$c_{\pm 3}$	$3k \rightarrow \exp(3ikx)$	$3\hbar k$
$\vdots$		

**Table 1:** Coefficients of the wave function. If we plot the position probability density, longitudinal and transversal pump might look quite similar. We thus perform a Fourier transform so we can access the  $c_l$ 's and gain further insight into the physical system. For longitudinal pump, we only expect  $c_0, c_{\pm 2}, c_{\pm 4}, \dots$  while for transversal pump we expect  $c_0, c_{\pm 1}, c_{\pm 2}, c_{\pm 3}$  and so on.

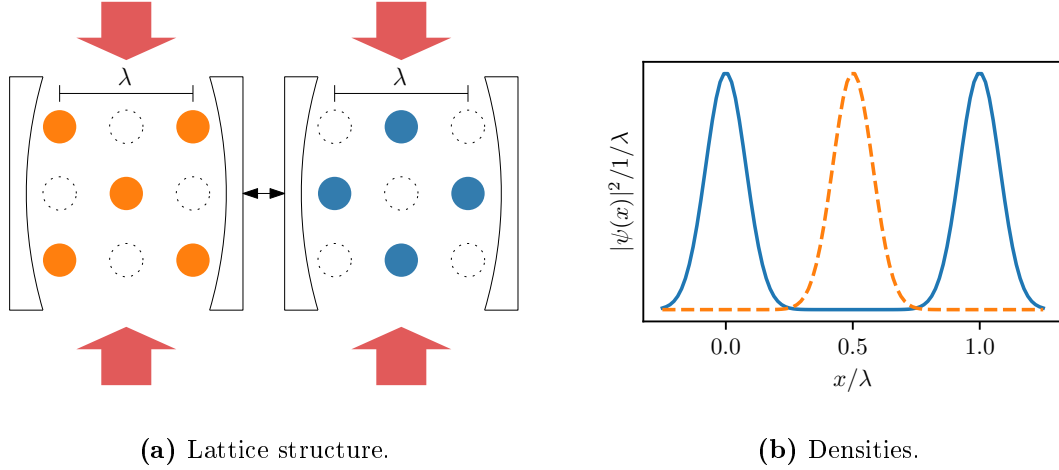
Figure 3 shows two Figures from a paper that investigates a Bose-Einstein condensate in a transversally pumped cavity [7]. On the right, we see what we're already familiar with: The peak of the position probability density is located at the lowest point of the potential. That atoms localize at the potential "valleys" to minimize their energy. On the left, there's an illustration of the order parameter  $\Theta$  versus the pump strength  $\eta$ . When  $\Theta = 0$ , the atoms are uniformly distributed in the cavity. When  $\Theta = 1$ , the atoms are in a lattice pattern. The interesting thing about transversal pump (which is also described in [1]) is that the atoms are initially resisting being ordered and suddenly arrange themselves in a lattice pattern depending on the pump strength. Initially,  $\Theta$  stays at 0. At a critical pump strength however, suddenly the order parameter jumps up. This is also a behavior which we expect to see in our simulations later.



**Figure 3:** Order parameter and lattice potential for transversal pumping. When we pump transversally, the atoms initially don't order themselves in a lattice. Only at a critical pump strength  $\eta_{\text{crit}}$ , self-organization takes place rapidly. The location of the atoms will be in the potential minima. Figures taken from [7].

Notice also that in Figure 3b, the wave function density and the potential are  $\lambda$ -periodic, as the Hamiltonian for the transversally pumped cavity is also  $\lambda$ -periodic.

As such, there are two ways in which the atoms arrange themselves inside the cavity, as depicted in Figure 4a. In our simulations, we will observe a  $\lambda/2$  periodicity. That is because we'll be looking at the superposition of two symmetric states that are just shifted by  $\lambda/2$ . Measuring the system experimentally, we would obtain only one state. That is also the case when investigating the system analytically, as in [7]. When we're doing simulations, however, it won't be possible for us to separate the two states. Figure 4b shows what we expect to see in the simulation.



**Figure 4:** Lattice configuration and superposition of densities. There are two ways for the atoms to arrange themselves, as shown on the left. If we were to measure the system experimentally, we'd only obtain one lattice pattern. In the simulation, however, we obtain the two configurations simultaneously, thus observing a  $\lambda/2$ -periodic position probability density.

To summarize, the expected properties of our systems are:

- The atoms are localized in the "valleys" of the optical potential.
- Longitudinal pumping:
  - The atoms can have momenta of  $2n\hbar k$ .
  - The more we pump, the more photons we will get.
- Transversal pumping:
  - The atoms can have momenta of  $n\hbar k$ .
  - There is an abrupt self-organization.
  - We observe a superposition of two symmetric states.

## 5 Simulation

Having derived our Hamiltonians, we'll now set out to numerically simulate the systems (more specifically, the ground state of our Hamiltonians). In the following sections, we'll present the code necessary to simulate the quantum systems. However, any code to generate graphs will not be presented.

## 5.1 The Julia language and QuantumOptics.jl

Scientific computing requires high performance which low-level languages like C or Fortran can deliver. However, writing scripts in these languages can often be cumbersome. Julia is a programming language that promises the ease of use of high level-languages and performance of low-level languages [8]. We won't go into further details whether that's true or not. So here we use Julia for our simulations. Then we have to ask ourselves how to represent the physical systems on the computer. We could program everything from scratch which everybody doing numerical simulations should probably do a couple times. However, after a while it gets redundant because we're doing the same things over and over again. We will thus use a framework which is called QuantumOptics.jl [9]. With that framework, a lot of functions are executed in the background and as such it's more convenient for us. The architecture of the functions of the package will not be discussed. A detailed documentation can be found at [10].

## 5.2 The Code

First, we'll add all the packages that we need:

```
using QuantumOptics, LinearAlgebra
```

The package `QuantumOptics` is the quantum simulation package mentioned earlier and `LinearAlgebra` is a package that comes with some useful functions like getting the diagonal entries of a matrix `diag()`. We'll set  $k = 2\pi$ , so that  $\lambda = 1$ . The recoil frequency we set  $\omega_r = 1$  and  $\Delta_c = -10\omega_r$  and  $U_0 = -1\omega_r$ :

```
k = 2*π  
ωr = 1  
Δc = -10 * ωr  
U0 = -1 * ωr
```

For now, we'll allow a maximum of  $N = 16$  photon states. Setting  $N_{\text{cutoff}}$  higher would increase the computational time. However, it might be necessary depending how much photons we have in the cavity which depends on the pumping strength  $\eta$ . The dangers of setting  $N_{\text{cutoff}}$  too low will be discussed in the results. We'll confine the simulation spatially to  $x_{\text{min}} = 0$  and  $x_{\text{max}} = 1$ . Setting a wider range would be redundant since the transversal Hamiltonian is  $\lambda$ -periodic. Usually, the step size is set to  $N_{\text{steps}} = 2^n$ , where  $n \in \mathbb{N}$ . Here, we set  $N_{\text{steps}} = 64$  for a good compromise between simulation time and the look of the graphs.

```
N_cutoff = 16  
xmin = 0  
xmax = 1  
Nsteps = 32
```

We define the bases, as well as the raising and lowering operators:

```

b_position = PositionBasis(xmin, xmax, Nsteps)
b_fock = FockBasis(N_cutoff)
p = momentum(b_position)
a = destroy(b_fock) ⊗ one(b_position)
ad = dagger(a)

```

The raising and lowering operators are a tensor product of the position and Fock basis. Note that in Julia it's possible to name variables with Greek symbols. In this case, the tensor product is defined with the symbol  $\otimes$ . We define the Hamiltonian and calculate the first three states with  $\eta = 30\omega_r$ :

```

η = 30 * ωr
potential = x -> U0*cos(k*x)^2
H_int = (one(b_fock) ⊗ potentialoperator(b_position, potential))*ad*a
H_kin = (one(b_fock) ⊗ p^2) / k^2
H_cavity = -Δc*ad*a
H_pump = η*(a + ad)
H = dense(H_int) + H_kin + H_cavity + H_pump

E, ψ_states = eigenstates((H + dagger(H))/2, 3)

```

Notice that in the last line, instead of  $H$  we use  $(H + \text{dagger}(H))/2$  to make the Hamiltonian truly Hermitian. Due to numerical errors, the operator  $p^2$  is not Hermitian here. If we want to plot the wave function, we'll have to extract the position part of the composite basis. We can do that with the command `ptrace()`. We thus obtain a matrix whose diagonal entries are the complex values of the wave function:

```

pos_dense = ptrace(ψ_states[1], 1)
density = diag(pos_dense.data)

```

We need to add the suffix `.data` to extract the values of `pos_dense`. Otherwise, we'd get an error since the function `diag()` cannot take objects defined by the quantum optics framework. By changing the second argument of `ptrace()` to 2, we trace out the position basis. The diagonal entries of the obtained matrix represents the photon number distribution:

```

photon_dense = ptrace(ψ_states[1], 2)
probab = diag(photon_dense.data)

```

We can calculate the expected photon number as follows:

```

ada_exp = expect(ad*a, ψ_states[1])

```

We can also calculate the momentum distribution which is the Fourier transform of the position distribution. The function `transform()` performs a Fourier transform in the background:

```

b_momentum = MomentumBasis(b_position)
Tpx = transform(b_momentum, b_position)

pos_dense = ptrace( $\psi$ _states[1], 1)
states_p = Tpx * pos_dense
density_p = diag(states_p.data)

```

Now let's tackle the transversal pump. The bases are the same as before. However, we have to define different Hamiltonians:

```

 $\eta$  = 10 *  $\omega$ r
potential = x -> U0*cos(k*x)^2
H_int = (one(b_fock)  $\otimes$  potentialoperator(b_position, potential))*ad*a
H_kin = (one(b_fock)  $\otimes$  p^2) / k^2
H_cavity = - $\Delta$ c*ad*a
pump = x ->  $\eta$ *cos(k*x)
H_pump = (one(b_fock)  $\otimes$  potentialoperator(b_position, pump)) * (a + ad)
H = H_kin + dense(H_int) + H_pump + H_cavity

E,  $\psi$ _states = eigenstates((H + dagger(H))/2, 3)

```

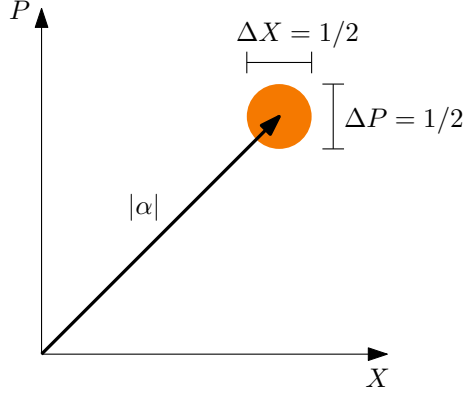
To visualize the degree of self-organization, we'll take a look at the photon state. The Husimi Q representation is a way of visualizing a wave function. It's defined as follows:

$$Q(\alpha) = \frac{1}{\pi} \langle \alpha | \rho | \alpha \rangle, \quad (28)$$

where  $|\alpha\rangle$  is the state we want to visualize and  $\rho$  is the density operator of the photon state:

$$\rho = |\psi\rangle\langle\psi|. \quad (29)$$

In our case,  $|\alpha\rangle$  is a coherent state. It is represented by a dimensionless complex number  $\alpha = X + iP$ . The Q-Function is a quasiprobability distribution. For every possible value of  $\alpha$ , i.e. for every point on the  $X - P$ -plane the Q-Function will give us the probability of that state. Figure 5 shows a coherent state in phase space.



**Figure 5:** Coherent state  $|\alpha\rangle$  in phase space. The state  $|\alpha\rangle$  is represented by a dimensionless complex number  $\alpha = X + iP$ . To each axis, there is a quantum uncertainty of  $1/2$ .

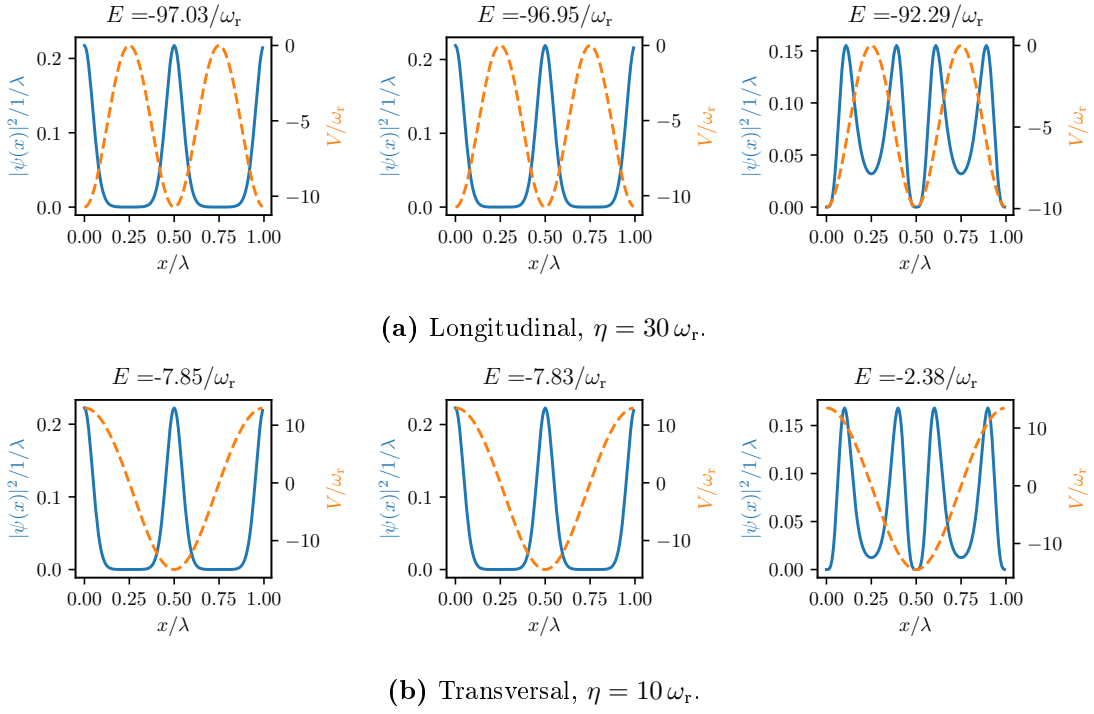
In Julia with QuantumOptics.jl, we can use the command `qfunc()` to get the Husimi Q representation of the photon state:

```
bdr = 6
xvec = [-bdr:.1:bdr;]
yvec = [-bdr:.1:bdr;]
photon_dense = ptrace( $\psi\_states[1]$ , 2)
grid = qfunc(photon_dense, xvec, yvec)
```

The variable `bdr` was set heuristically for plotting.

## 6 Results and Discussion

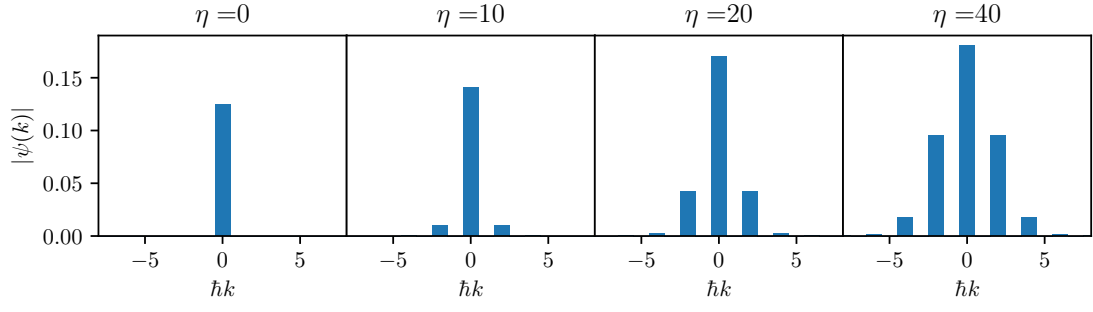
The position probability densities can be seen in Figure 6. On the top, there's the longitudinal pump and on the bottom the transversal. The leftmost state is the first eigenstate, the second eigenstate is in the middle and the third on the right. The first eigenstate has the lowest energy. The solid blue lines represent the position probability densities, the dashed orange lines represent the potentials. The potential plot was created by taking the expressions of the respective Hamiltonians that act both on the atom part and the photon part of the composite system. For the operators the expectation values were taken. Each peak of the ground state density being located at the potential minima is in accordance with our expectations. Notice that the transversal position probability density is  $\lambda/2$ -periodic despite the Hamiltonian being  $\lambda$ -periodic. This is because we're actually looking at the superposition of two symmetric states that are shifted by  $\lambda/2$ . There'd be actually two potentials in Figure 6b, one for each state. However, only one was chosen so that the graph doesn't get too confusing. The other potential would look the same, but shifted by  $\lambda/2$ . The position probability densities give us an idea where the atoms are located. There are some properties of the systems, however, which still remain hidden to us in this representation. For that, we'll take a look at the momentum space.



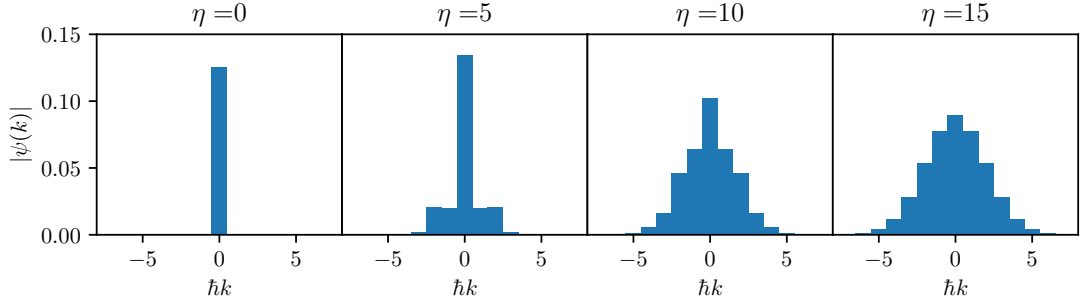
**Figure 6:** Longitudinal and transversal position probability densities. The solid blue lines represent the position probability densities and the dashed orange lines represent the potentials. The first eigenstate is on the left, the second in the middle and the third on the right. The wave function densities being located at potential minima meets our expectation. Note that the transversal position probability density appears to be  $\lambda/2$ -periodic. That is because we're actually looking at the superposition of two symmetric states that are shifted by  $\lambda/2$ .

The momentum distribution for different values of  $\eta$  can be seen in Figure 7. At  $\eta = 0$ , i.e. when the laser is off, there's only a peak at 0, meaning the atoms have no momentum. When we start pumping, we get other peaks than 0. Now the atoms do have momentum. For longitudinal pumping, there's always a gap between each peak which is not the case for transversal pumping. Take a look again at figure 2. When we pump longitudinally, a photon is only able to transfer a momentum of  $2\hbar k$  because of momentum conservation. Thus we only observe peaks at  $2n\hbar k$ , where  $n \in \mathbb{N}$ . For transversal pumping, the same processes of photons transferring momenta of  $2\hbar k$  are happening, but now we also have a momentum transfer of  $\hbar k$  when a transversally incoming photon is being scattered into the cavity. Naturally, the more we pump, the more outer momenta we will get.





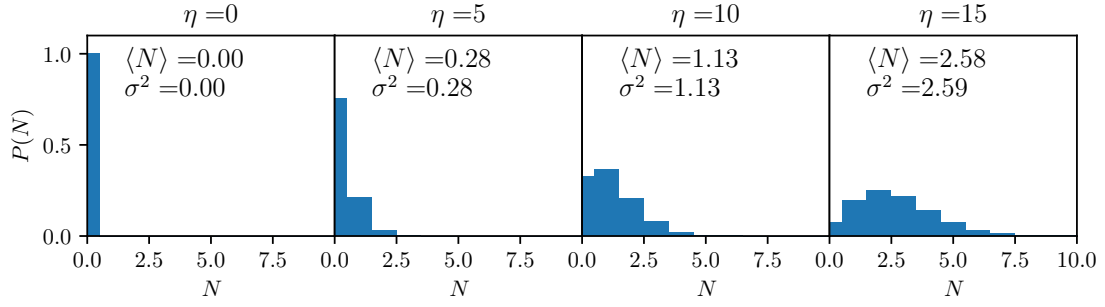
(a) Longitudinal.



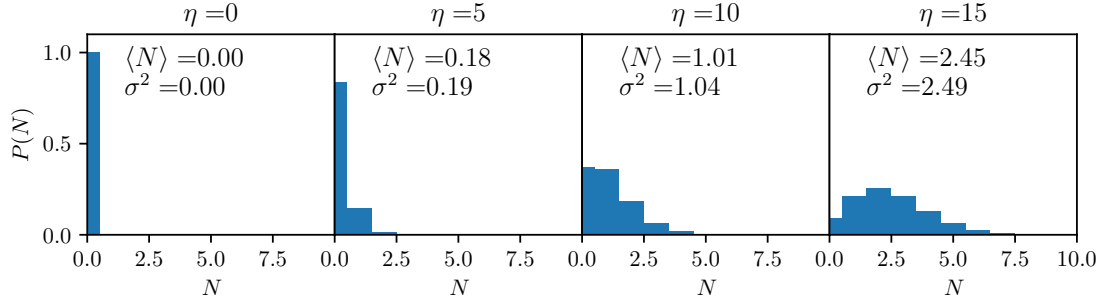
(b) Transversal.

**Figure 7:** Longitudinal and transversal momentum distributions. For longitudinal pump, there are only momenta of  $2n\hbar k$  because longitudinal scattering processes only allow momenta transfer of  $2\hbar k$ . For transversal pump, there is no such restriction and we have momenta of  $n\hbar k$ .

Having looked at the atom part of the composite system, let's take a look at the photon part. The photon number distribution for different values of  $\eta$  can be seen in Figure 8. The mean and variance are the same, thus we have a Poisson distribution.



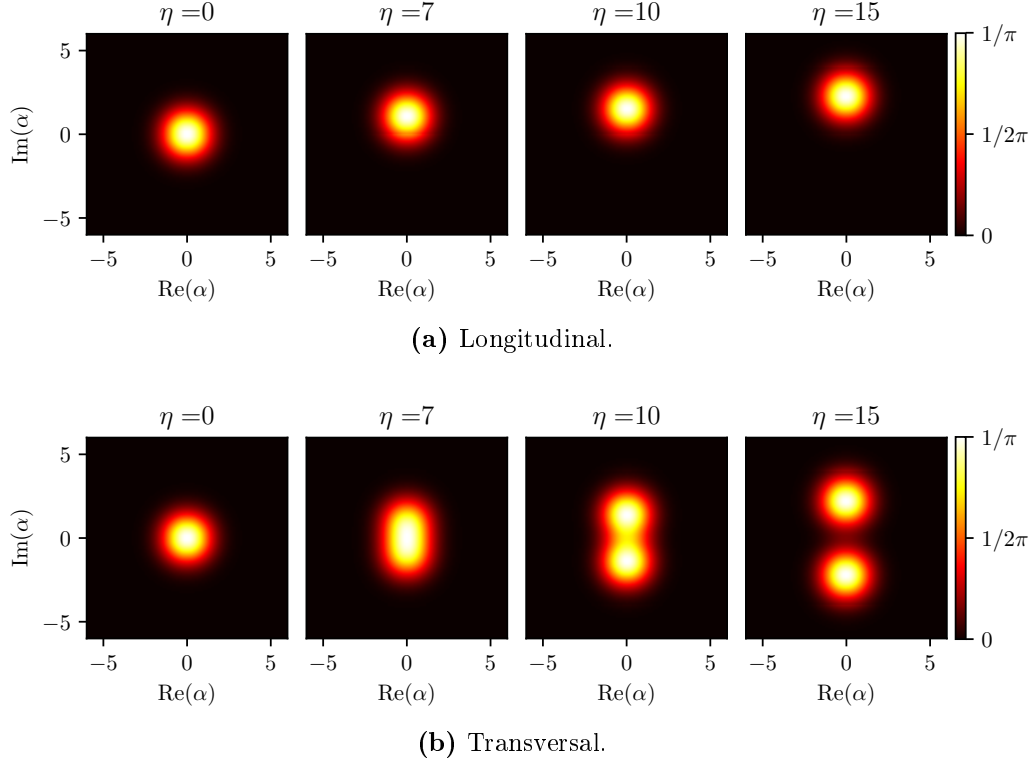
(a) Longitudinal.



(b) Transversal.

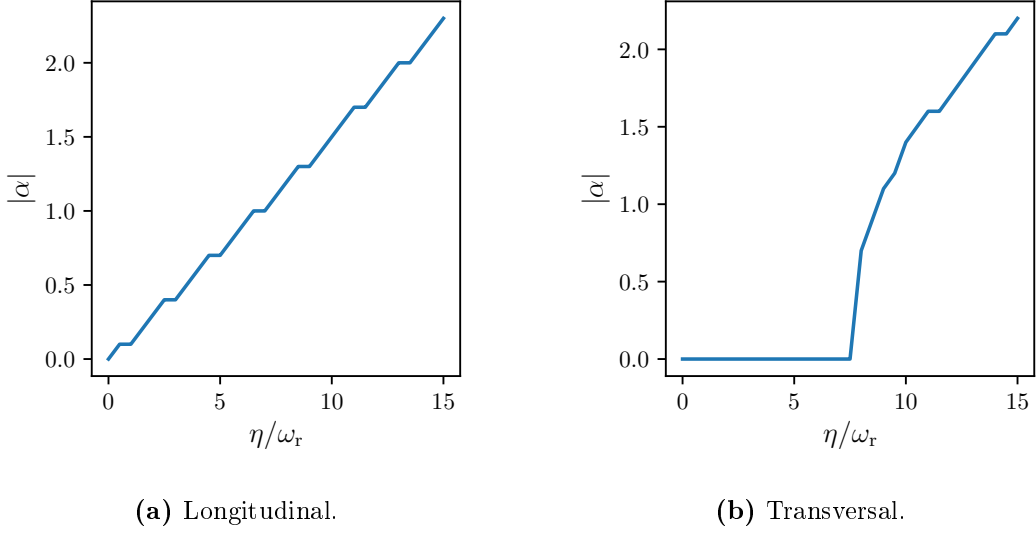
**Figure 8:** Longitudinal and transversal photon distributions. Since the mean and the variance are the same, we have a Poisson distribution.

The Humsimi  $Q$  representation of the photon states for longitudinal and transversal pump can be seen in Figure 9. What we can see is a two-dimensional plane. A point on this plane represents a state the light field can be in. Remember that the state  $|\alpha\rangle$  is represented by a complex number  $\alpha = X + iP$ . We don't only see a point, however, we can see a blob. That is because of the quantum uncertainty. The color represents the probability of a certain state, white is the highest probability and black 0. Taking a look at the longitudinal case, the blob is initially at 0 meaning that there's no light field. There more we pump then, the higher the blob will move which indicates the emergence of a light field. A light field being present means of course the atoms being arranged in a lattice. For the transversal pump, the graphs look a little different. First of all, we can observe two blobs. That is because we're looking at the superposition of two symmetric states that we can't separate in the simulation. Then notice also that initially the blob in the middle doesn't separate into two, but stretches with the highest probability of the state still being at 0.



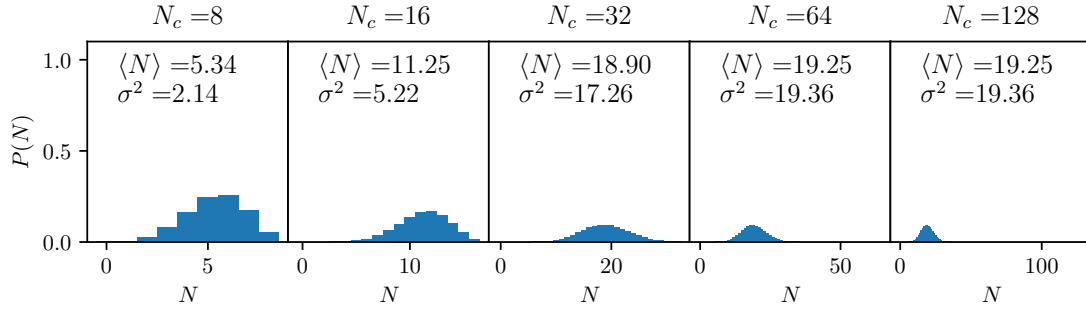
**Figure 9:** Husimi Q representation of photon states for longitudinal and transversal pumping. A point in the plane represents a state  $|\alpha\rangle$  of the light field and the color the probability of that state. Since there's quantum uncertainty, we don't observe a point but a blob. For transversal pumping, the blob initially doesn't move but only stretches. Only at sufficient pump strengths, the blob will move and thus a light field build up. Observing two blobs for transversal pumping means we're actually looking at the superposition of two symmetric states.

We can visualize the fact that the two blobs initially don't separate but only stretch by plotting the pump parameter  $\eta$  on the  $x$ -axis and the most likely state for one half of the plane on the  $y$ -axis which is effectively the absolute value of  $\alpha$ . We can see the result at Figure 10. For longitudinal pumping, the more we pump, the more light field will build up, i.e. there is a direct relationship between pumping and light field intensity. For transversal pumping we can see another picture, however. Initially when we pump, the graph stays at 0 meaning no light field is building up. Only at a critical pump strength, a light-field will suddenly emerge. This is what we have discussed earlier about the sudden face transition for the transversal pumping.



**Figure 10:** Most likely value of the photon state momentum looking at only the positive side of the phase space for longitudinal and transversal pumping. For longitudinal pumping, the momentum increases gradually. For transversal pumping, the light initially does not gain any momentum, meaning that the atoms resist being in order. At a critical pump strength, a light field suddenly builds up and the atoms self-order.

The more we pump, the more photons will appear. We have to take that into account by raising the maximum amount of allowed photon states  $N_{\text{cutoff}}$ . Raising  $N_{\text{cutoff}}$  results in longer simulation times which can be bothersome. However, if we don't do so, our results become faulty. Take a look at Figure 11 which depicts the photon number distributions for longitudinal pump for different values of  $N_{\text{cutoff}}$  at  $\eta = 40\omega_r$ . For our parameters,  $40\omega_r$  is a relatively high value for  $\eta$  and we thus would expect a high average photon number which we cannot possibly obtain if we limit  $N_{\text{cutoff}}$  to 8. To check the validity of our results, i.e. if  $N_{\text{cutoff}}$  is set high enough, we can look at the standard deviation. For a Poisson distribution, the mean has to be the same as the standard deviation which is not the case if we set the cutoff too low.



**Figure 11:** Photon number distributions for longitudinal pump for different values of  $N_{\text{cutoff}}$  at  $\eta = 40\omega_r$ . If we don't set  $N_{\text{cutoff}}$  sufficiently high, we get bogus results. A quick sanity check is to compare the mean with the variance. For a Poisson distribution, they have to be the same.

## 7 Outlook / Conclusion

In this thesis, we asked ourselves the question how to arrange atoms in a lattice to simulate a solid. The reason we might want to do that is that on top of a naturally occurring solid being hard to look into, we can't change it, e.g. modify the lattice structure. Since atoms arranged in a lattice are able to represent a quantum system under certain conditions, we can use that quantum system to simulate another. Here we're stepping in the rapidly expanding field of quantum simulations. For those wishing to explore some of the recent advancements, [11] is part of a dossier with mini-reviews. In our case, we make use of light to trap atoms, more specifically lasers. If two laser beams are counter-propagating, the intensity will form a cosine pattern. Between those two lasers, there's our atoms. The special trick is to set the frequency of the lasers way below the excitation frequency of the atoms. That will induce a dipole in the atoms which will interact with the light field. Now we have a potential for the atoms and they will go to the lowest points to minimize their energy. To enhance atom-light field interaction, we put the atoms in a cavity. We looked at two ways to pump the cavity: longitudinally and transversally. The transversal pump has a couple special properties, one of which is the sudden phase transition: Initially, nothing happens when we pump and the atoms stay uniformly distributed. Then, at a critical pump strength, a light field will suddenly build up and the atoms be arranged in a lattice. In the programming language Julia with the framework QuantumOptics.jl we conducted a couple simulations which fulfilled our expectations quite neatly.

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