Collective effects of radiatively interacting ultracold atoms in an optical resonator

Ph.D. Thesis

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## Summary

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Chapter 1

Introduction

The nature of light has been of central interest since the earliest days of science. Many of the great scientists devoted their time to improve our understanding of light. Long after the speculations of the Greek philosophers, the first milestone work emerged interestingly in the Islamic world nearly thousand years ago. The *Book of Optics* was written in 1021 by the Arab polymath Ibn al-Haytham. Besides explaining the process of vision, he laid down the principles of optics on an experimental basis, that gained him the title of “father of modern optics.” Seven centuries had to pass in Europe until the birth of Newton’s theory of colour published in the remarkable treatise “*Opticks*” appeared in 1704. The following important stage was Maxwell’s paper from 1864, in which he established the basis of classical electrodynamics. Einstein himself had been captivated by the mystery of light since his youth. His simple explanation of the photoelectric effect in terms of “light quanta” in 1905 revealed the fundamental character of light. In 1917, it was also Einstein, who first made a distinction between spontaneous and induced quantum processes, which laid ground not only for lasing, but for the laser manipulation of atoms. The picture became complete in 1927, when Dirac quantized the electromagnetic field, and calculated the Einstein coefficients, establishing quantum electrodynamics.

For centuries, optics was dealing with light-matter interactions from the viewpoint of light. Matter was only used to tailor the propagation or the spectrum of light, whereas its properties were simplified and taken into account as a refractive index. The development of the laser in the 1960s made possible the opposite situation. By the repeated scattering of photons being in the same quantum state, coherent manipulation of matter with light became possible. This advanced tool revolutionized atomic physics, which was a flourishing field by that time. Lasers enabled physicists to precisely measure and manipulate not only the internal state of atoms (with laser spectroscopy and optical pumping), but also their motional degrees of freedom.
1.1 Laser cooling and trapping

In the optical domain, photons have large enough momentum to considerably modify the atomic motion. Scattering of one photon yields generally a few cm/s change in the velocity of alkali atoms. In an intense laser field, the rate of inelastic photon scattering is determined by the spontaneous emission rate of the atom, that amounts to an acceleration about $10^5$ times larger than the gravitational acceleration on Earth. Accordingly, a collimated thermal atomic beam can be ‘stopped’ by a counter-propagating laser beam within a few tens of centimeters, first demonstrated by Phillips and Metcalf in 1982 [1]. Following the proposal of Hänsch and Schawlow [2], Chu was able to cool the slow atoms further by exploiting the Doppler effect in 1985 [3]. In the Doppler cooling scheme the atoms are illuminated from all directions by lasers whose frequency is detuned slightly below an atomic resonance line. Then, the Doppler-shift pulls the beams opposing the atomic motion closer to resonance and pushes the co-propagating beams farther from resonance, hence the atom is more likely to absorb photons with momentum opposite to its motional direction. On average, the inelastic photon scattering yields a nonlinear friction force, which can be linearized for slow velocities resulting in a viscous damping.

The three pairs of counter-propagating laser beams create a photon sea that acts like an exceptionally viscous fluid, literally called “optical molasses”. Treating the atoms as pointlike particles, they undergo classical Brownian motion [4]. Besides friction, they experience momentum diffusion as well arising from the random kicks of the spontaneously emitted photons. According to the Einstein relation, the equilibrium temperature of the atomic cloud is determined by the competition of these two effects. The lowest achievable temperature scales with the linewidth of the atomic transition and it is realized at a frequency of half linewidth below resonance. For alkali atoms this so-called Doppler temperature is on the order of 100µK.

After the cooling stage, the next challenge was to confine the roaming atoms inside a trap. The pioneer of optical trapping was Ashkin, who first demonstrated the acceleration and trapping of micron-sized latex spheres in water with focused laser beams in 1970 [5]. His invention, the optical tweezer [6], which is suitable to trap and move microscopic objects (even an individual virus or a living bacterium), became widely used in biophysics. Furthermore, with Gordon he examined the possibility of trapping atoms in a radiation trap by describing the light forces, including their dependence on the atomic velocity and quantum fluctuations [7]. They identified the two types of forces acting in a laser field: the scattering (or radiation pressure) force, that they associated with absorp-
tion followed by spontaneous emission, and the dipole force originating in the coherent redistribution of photons due to stimulated emission. They showed that unlike the scattering force, the dipole force is conservative, and the corresponding optical potential is proportional to the field’s intensity. Moreover, its sign depends on the detuning between the laser frequency and the atomic resonance. When the laser is tuned below resonance (red detuning) the optical potential is negative, hence the atoms are attracted towards the high intensity regions of the field, behaving as high field seekers. However, for blue detuning the potential is positive, so the atoms are repelled out of the high intensity regions becoming low field seekers. Surprisingly, the dipole force vanishes on the atomic resonance\(^1\).

Since Ashkin’s first proposal [8] in 1978, a wide variety of dipole traps have been developed, and they became standard tools for manipulating and trapping cold neutral atoms [9]. The remarkable idea of the far-off-resonance trapping (FORT) made possible to suppress spontaneous emission to a negligible level by increasing the atom–laser detuning along with the field intensity [10]. The creation of highly conservative optical potentials with far-off-resonant laser beams opened up the way to “atom optics”, the coherent manipulation of atomic matter waves with light [11].

In contrast to the long-term success of the dipole traps, in the beginning they failed to collect the majority of atoms (\(10^3\) out of \(10^6\)) from the optical molasses because of their small trapping volume. The first robust trapping scheme was realized in 1987 [12], following the idea of Jean Dalibard. The magneto-optical trap (MOT) uses the radiation pressure force for combining Doppler cooling with magneto-optical trapping. As the force is velocity dependent due to the Doppler shift, it can be also made position dependent through the Zeeman shift produced by a magnetic field gradient. If one has two red-detuned counter propagating laser beams of opposite circular polarizations and a magnetic field that changes sign at the center, then different Zeeman sublevels are pulled closer to resonance preferring absorption from opposite beams at opposite sides. Thus, one can set the parameters so that the atoms being right to the center would preferably absorb photons from the beam coming from the right and the atoms on the left would

\(^1\)This intriguing nature of the dipole force can be easily understood from classical physics. The oscillating electric field \(\mathbf{E}\) induces an atomic dipole moment \(\mathbf{d}\), that can be considered a driven damped harmonic oscillator. In this manner, the optical potential is created by the dipole interaction energy \(\mathbf{d}\mathbf{E}\), that varies in space. An oscillator driven below its resonance responds in phase with the driving field, resulting in negative interaction energy, whereas an oscillator driven above its resonance oscillates out of phase with the driving, yielding positive interaction energy. On resonance, the oscillator is 90 degrees out of phase, hence the interaction energy cancels out on time average over the optical period.
dominantly absorb photons from the left beam, that results in a net force pointing to the center. In three dimensions, with an anti-Helmholtz magnetic field superimposed on the optical molasses, a restoring force can be created, which pushes the atoms towards the centre of the trap, where the magnetic field is zero. Because of its simultaneous cooling and trapping facility, the MOT has become a widespread source of laser-cooled atoms, that is capable to cool and hold up to $10^{10}$ atoms within a trapping volume of about one cubic centimetre.

Strikingly, much lower temperatures were detected in the MOT than the Doppler limit, which initiated the finding of a new type of cooling process, the so-called polarization gradient cooling [13]. It emerges from the delicate combination of two effects: optical pumping and AC Stark shift. Optical pumping is suitable to create a one-way transition between different ground state Zeeman sublevels by circularly polarized laser light. Whereas, AC Stark shift is the splitting of the atomic Zeeman sublevels in the oscillating electric field of a non-resonant optical excitation. Both effects depend on the polarization of light. Generally, in a MOT, laser polarization varies in space between different linear and circular polarizations, and the light shifts of the sublevels vary accordingly, giving rise to distinct periodic optical potentials for distinct sublevels. Cooling is possible when optical pumping transitions take place from higher to lower potential energies. In this case, a moving atom continually climbs potential hills at the expense of its kinetic energy, because at the top of the hills it is pumped down to a lower energy spin state. After the famous figure of the Greek mythology, this kind of cooling process was christened Sisyphus cooling. Succeeding the Doppler cooling, it could slow the atoms down to the recoil temperature, which corresponds to the energy scale of the recoil due to the absorption or the emission of a single photon. For alkali atoms, the recoil temperature is on the order of $1\mu K$.

One might think that this is the fundamental limit of laser cooling, since the last spontaneously emitted photon would result in a random velocity of this magnitude. Nevertheless, it is still possible to circumvent it with more sophisticated methods like velocity-selective coherent population trapping [14] and Raman cooling [15]. By applying these techniques, the temperature of the atoms could be lowered by three orders of magnitude, down to the nanokelvin range in the mid-1990s [16, 17]. These methods have no strict cooling limits, however, the accompanying large atom loss gives a lower bound on the temperature and an upper bound on the achievable atom density.

For further reviews on laser cooling, consult the Nobel lectures of C. Cohen-Tannoudji [18], S. Chu [19] and W. D. Phillips [20].
1.2 Bose-Einstein condensation

By the early 1990s, the quest for Bose-Einstein condensation in a dilute atomic gas had become a central goal of the atomic physics community.\cite{[21, 22]}. The most important benefit of diluteness is in the reduction of the interparticle interactions, which normally precludes a gas from reaching quantum degeneracy. Cooling a dense gas would lead to a liquid, then a solid, whereas cooling a dilute gas can lead to a metastable phase, that is defined by quantum statistics.\footnote{The only exception is He\textsuperscript{4} which remains a liquid even at zero temperature, and it becomes a superfluid below 2.2 Kelvin. For half a century it was the sole realization of Bose-Einstein condensation, however it is a strongly interacting system with a condensate fraction less than 10\%.} In fact, the density tunes the ratio between two- and three-body collisions among the gas particles. At sufficiently low densities, the three-body recombination — being responsible for molecule formation — is highly suppressed in favour of the two-body collisions that are essential for reaching thermal equilibrium. For instance, at typical experimental densities being on the order of 10\textsuperscript{14} cm\textsuperscript{-3}, the lifetime of the metastable quantum gas is a few tens of seconds, which anyway, seems like an eternity on the timescale of the atomic processes.

In a simplified picture, the quantum nature of a gas shows up when the wave packets of its particles overlap. The size of the wave packets, in turn, is approximately given by the de Broglie wavelength of the particles, which is inversely proportional to their thermal velocity, hence to the square root of the temperature. Therefore, the critical temperature of the Bose-Einstein transition scales with the particle density, \textit{i.e.}, it is lower for a more dilute gas. At such low densities required by metastability, it ranges from ten nanokelvin to ten microkelvin, that usually raises need for subrecoil cooling.

Despite of the amazing development of laser cooling, quantum degeneracy could not be reached solely by its means. However low temperatures could be produced with sub-recoil cooling, the accompanying atom loss precluded to obtain high enough phase space densities. The other route to degeneracy, \textit{i.e.} increasing the atom number in a MOT at a constant temperature, also failed. Above a critical density, instabilities occured due to the attenuation of the laser beams and the multiple scattering of spontaneously emitted photons within the sample\cite{[23]}.

Meanwhile, several experimental groups made efforts to Bose condense spin-polarized atomic hydrogen gas using traditional cryogenics combined with magnetic fields. They made a breakthrough by applying evaporative cooling in a magnetic trap, a method proposed by Hess in 1986\cite{[24]}, and by 1991 they obtained phase space densities within a
factor of 5 of condensing. Cooling by evaporation is a straightforward way to decrease the temperature of a trapped interacting atomic gas. By merely letting the highest-energy atoms escape from the trap, the mean energy of the remaining atoms decrease, hence the gas gets colder, and its density increases – so it becomes compressed both in real and in momentum space. This can be continued as long as the remnant thermalizes itself at the new temperature, therefore two-body collisions play a key role in the process.

Ultimately, the successive combination of laser cooling and evaporative cooling proved to be the most efficient technique for creating ultracold quantum gases. The large, few hundred μK cold atomic samples produced in a MOT could be easily loaded into a spatially superimposed magnetic trap, which provided an excellent container for spin polarized atoms [25], thus it served as a good platform for further cooling by evaporation. Using these techniques, the first achievements of Bose-Einstein condensation in dilute alkali gases were made in 1995 by Cornell and Wieman with rubidium [26] and by Ketterle with sodium atoms [27]. Amazingly, the condensate fraction reached almost hundred percent in the experiments, meaning that a pure quantum matter was formed.

The physics of ultracold quantum gases has become a proliferating field in the last fifteen years [28]. As a reference, Bose-Einstein condensates (BEC) are routinely realized in more than fifty laboratories worldwide for a large variety of isotopes including mainly alkaline and alkaline earth atoms: \(^7\)Li, \(^{23}\)Na, \(^{41}\)K, \(^{84}\)Sr, \(^{85}\)Rb, \(^{87}\)Rb, \(^{133}\)Cs and a few others like \(^1\)H, \(^4\)He, \(^{52}\)Cr and \(^{174}\)Yb [29]. Degenerate Fermi gases are also created from \(^6\)Li and \(^{40}\)K opening up new research directions [30]. The attractiveness of ultracold quantum gases stems from their simplicity, controllability and generality. First, they are relatively easy to produce, maintain and manipulate in various forms. Second, their parameters are flexible, highly controllable, and there exist powerful methods to measure them. For instance, both the sign and the strength of the atom–atom collisions can be tuned by an external magnetic field \textit{via} the so-called Fesbach resonances [31]. Third, the understanding of these systems requires interdisciplinary physics including nonlinear and quantum optics, atomic and solid-state physics. Bose-Einstein condensates can be considered as coherent atomic de Broglie waves obeying a nonlinear wave equation, thus they show interference properties familiar from nonlinear optics like four-wave mixing and soliton formation [32]. By coupling out atoms from a trapped BEC, one gets a coherent source of matter wave, \textit{i.e.} an atom laser [33, 34]. Furthermore, ultracold gases are good quantum simulators for a number of models in solid-state physics. As an example, BCS (Bardeen-Cooper-Schrieffer) pairing can be studied experimentally in an ultracold Fermi gas with variable interactions [35]. More interestingly, for repulsive interactions diatomic
molecules can form from the fermionic atoms, which in turn are bosons, hence can be Bose condensed. The crossover between this molecular BEC and the atomic BCS state is a subject of current research [30]. As another example, artificial perfect crystals, or so-called optical lattices can be made by filling the atomic gas into the periodic optical potential created by standing wave laser fields. This system realizes the “clean” Hubbard model for either bosonic or fermionic particles in one, two, or three dimensions, hence it is able to show quantum phase transitions, e.g. the superfluid–Mott transition [36].

1.3 Cavity quantum electrodynamics

At the end of the last century, technology gave another gift to physicists, namely the high-quality optical resonator which proved to be a new precious element in experimental quantum optics. Cavity Quantum Electrodynamics (CQED) has not only opened up conceptually new ways in the manipulation of atomic internal and external degrees of freedom, but also created a new microscopic system consisting of a single atom and a single photon, the so-called atom-photon molecule.

Historically, CQED emerged from the simple idea that the radiative properties of a dipole can be modified by tailoring the mode density of the surrounding electromagnetic field. In 1946, Purcell pointed out the enhancement of spontaneous emission rates for nuclear magnetic moment transitions in the presence of a resonant electric circuit [37]. Forty years later, the Purcell effect was demonstrated experimentally for excited atoms traversing a microwave cavity. Tuning the cavity, spontaneous decay from the excited state could be either enhanced or inhibited by a few percent [38, 39, 40].

These early experiments were performed in the perturbative regime of CQED, where the resonator was merely used to modify the mode density of the electromagnetic vacuum. The dynamics of the cavity field was irrelevant, since both the atoms and the photons left the volume of the cavity too fast for further interaction. In the mid-1990s, however, the so-called strong coupling regime was achieved, in which the single-photon Rabi frequency describing atom-field coupling exceeded the rate of cavity decay and that of atomic spontaneous emission and the inverse of the interaction time. This means that the atom and the cavity field exchange an excitation many times before it is dissipated into the environment, or before the atom leaves the cavity.

At this point, an analogy with the formation of a diatomic molecule can be invoked, where the exchange of a valence electron leads to binding and non-binding molecular states. Similarly, in case of strong coupling, the atom and the field lose their identities and
create a new object, an atom-photon molecule [41], with an energy spectrum displaying a clearly resolved normal-mode splitting. The lower levels describe atom-photon binding, whereas the upper levels correspond to the repulsion of the atom out of the cavity volume. Slow excited atoms are indeed attracted [42] or repelled [43] by the vacuum field of the cavity, when either the photon energy or the atomic energy dominates the other one, respectively. The situation is opposite in the case of a ground state atom interacting with a cavity containing a single photon. This frequency dependent behaviour calls the dipole force into our mind, which we know from laser cooling. Indeed, this is the same force originating from the energy of the induced atomic dipole in the cavity field.

Strong coupling was first achieved in 1996 by Haroche in the microwave regime with a resonator built from superconducting niobium mirrors. The cavity field was coupled to excited states of highly-excited (so-called Rydberg) atoms flying through the cavity with thermal velocity. A series of fundamental quantum mechanical experiments were performed on the atom-photon molecule. For instance, the appearance of discrete frequency components in the spectrum of energy exchange between an atom and a weak coherent field inside the cavity provided a direct proof of field quantization [44]. In another exciting experiment, a measurement process was simulated by atoms traversing the cavity, which contained a superposition of coherent states. The measurement-induced quantum decoherence of Schrödinger cat states was observed quantitatively [45].

In the optical domain, strong coupling was made possible by the development of dielectric multilayer mirrors. So as to obtain high enough intracavity field, the short wavelength has to be compensated with small mode volume. However, as the distance between the mirrors is reduced, the number of photon reflections increases, therefore extremely good mirrors are needed for keeping down the cavity decay. In a typical experimental setup, the cavity length is below 100µm, and the reflectivity of the mirrors is higher than 0.99999, resulting in a finesse between $10^5$–$10^6$. Pictorially, this means that a photon bounces up to $10^6$ times between the mirrors before exiting the system.

High-quality optical resonators signify a breakthrough in the study of light-matter interactions which is comparable to the appearance of the laser. While in a laser field, strong interaction is obtained by the scattering of many identical photons on the atom, in a cavity, strong coupling is reached by the recycling of the same photon that impinges on the atom several times. This picture also explains the main difference, that is the backaction of the atoms on the light, which is negligible for a laser field, but essential in a cavity. The high number of photon round trips enhances the sensitivity of the resonator to an unprecedented level, which for example allows the detection of individual atoms.
falling through the cavity [46]. In fact, the optical resolution being half a wavelength in free space is improved proportionally to the square root of the round trip count. Thus, the escaping photons give a unique way to monitor single atom trajectories inside the cavity. In the atom-cavity microscope realized in 2000 [47, 48], a few micrometers spatial resolution has been achieved from the microsecond-resolved analysis of the transmitted field intensity.

The other novel aspect of atom-cavity interaction in optical resonators is the mechanical force acting on the atomic center-of-mass motion. As previously discussed at laser cooling, optical photons carry large enough momentum to exert appreciable light forces. We have distinguished two types of them, the radiation pressure force originating in photon absorption, and the dipole force arising from the coherent scattering of photons between radiation modes *via* induced emission. Both of these forces have diffusion through the fluctuations of the atomic dipole. In addition, spontaneous emission gives rise to a third, so-called recoil diffusion deriving from the atomic recoils induced by the randomly emitted photons. In an optical cavity, these forces are highly tunable, however, in a non-trivial manner, for example *via* suppressing or enhancing spontaneous decay. In contrast to a laser field – where a static optical potential can be assigned to the dipole force –, the cavity provides a dynamic optical potential, which depends on the atomic motion. Furthermore, the field of the resonator fluctuates due to the photon leakage through the mirrors, which yields an additional diffusion force. Finally, for depicting the strength of the interaction, let us emphasize that in the atom-cavity microscope [47, 48] single cavity photons were able to bind in orbit single atoms for up to a few milliseconds.

Strong coupling in the optical domain was first attained in 1998 by the Kimble group (Caltech) [49] and a year later by the Rempe group (MPQ Garching) [50]. As an initial step, these CQED experiments used laser cooling techniques for producing a cold atomic sample. Typically, a large number of atoms (about $10^7$) are collected in a MOT, and some of them are dropped out or kicked out with a laser towards the cavity volume at a velocity of a few meters per second. The cavity is either pumped directly with a laser beam *via* one of its mirrors (cavity pumping), or fed by coherent scattering on the atoms from a laser that is perpendicular to the cavity axis (so-called atomic or transverse pumping). This latter scheme has the advantage that it solves three problems simultaneously. Besides the feeding of the system, a transverse slowly moving laser standing wave can also serve as an optical conveyor belt [51] that is suitable to optically transport single atoms from the MOT into the cavity [52]. In addition, the laser field provides an optical dipole trap in the transverse direction, hence, with two transverse beams together with the field of
the cavity, three dimensional trapping of a single atom has been achieved \cite{53, 54} for trapping times up to 17 seconds \cite{55}.

Optical cavities can trap atoms for long times if they are exploited for atom cooling. What the MOT realizes for a large number of atoms, the optical resonator attains for a single atom, \textit{viz.} simultaneous cooling and trapping. Generally, cooling means the irreversible damping of the atomic kinetic energy through coupling to the environment. In laser cooling, the atomic center-of-mass motion is coupled to the surrounding vacuum modes \textit{via} inelastic scattering of laser photons, thus dissipation manifests itself through spontaneous emission. In the perturbative regime of CQED (for weak atom-photon coupling), the cavity can be used as a spectral filter to modify the mode density of the electromagnetic field around the atomic resonance. In such a coloured vacuum, those scattering processes can be favoured in which the photon frequency is converted upwards taking away kinetic energy. Based on this concept, a number of cooling methods have been developed at the dawn of optical CQED \cite{56, 57, 58, 59}. As a matter of fact, in these techniques the resonator remains a passive element that is used to improve or generalize laser cooling schemes only having the dissipative channel of spontaneous emission.

In the strong coupling regime of CQED, a novel cooling mechanism takes place \cite{60, 61, 62, 63}. The atom is so strongly coupled to a given mode of the cavity that they share all dissipation channels of the system. Then, the atomic kinetic energy can be dissipated through the photon loss channel of the cavity mode. For adequately chosen detunings, cooling arises from the coupled atom–field dynamics. Astonishingly, the dipole force – which is conservative in a laser field – can result in a velocity dependent friction force in the cavity. This is because the motion of the atom acts back on the field by modulating the cavity resonance. Hence, the field creates a dynamic optical potential whose depth depends on the atomic position. However, the field follows the atom’s motion with a delay that corresponds to the cavity relaxation time. Therefore, the atom encounters a retarded optical potential, and the amount of retardation depends on its velocity. Besides the dissipation, diffusion also emerges in the system in agreement with the fluctuation-dissipation theorem. Pictorially, the optical lattice fluctuates due to the photons leaking out of the cavity, that heats the atom. Spontaneous emission plays no role in this cooling process, it can even be eliminated for large enough atom–pump detuning. In this case, the final temperature is determined solely by the photon loss channel of the cavity, and – in analogy to free-space laser cooling – it is proportional to the cavity mode linewidth. This can be smaller than the linewidth of the atomic transition, thus dynamical cavity
cooling can realize sub-Doppler temperatures. The first experimental demonstration was reported in 2003 [64], followed by a series of experiments with different parameters and geometries [65, 66, 55].

The most important benefit of cavity cooling is that it provides a general method to cool polarizable particles. As it uses the dipole force, no real optical excitations need take place, hence – in contrast to Doppler cooling – no closed optical cycle is necessary for the repeated scattering of photons. In the limit of large atom–laser detuning, the far-off-resonance trapping scheme can be generalized for the cavity field which can simultaneously trap and cool arbitrary polarizable objects [67]. In this wise, cavity cooling seems to provide a solution for the optical cooling of molecules, that is still a subtle open problem [68, 69].

Over recent years, the study of many-body phenomena in optical resonators has attracted considerable attention. For several atoms, light–matter interaction in the strong coupling regime is, by nature, a many-body problem. As all atoms are coupled to the same cavity mode, one of them feels the change in the field that is caused by the others. Thus, the field of the resonator mediates a long-range atom–atom interaction, which gives rise to interesting collective effects.

Although collective light forces in an optical resonator have been reported in the Rempe group as early as 2000, at that stage of the experiments it was difficult to trap more than one atom in the small cavity volume [70]. So as to observe many-body phenomena, the cavity mirrors were placed farther apart, and further magnetic or magneto-optical trapping was used to keep a large number of atoms inside the cavity. Extending the mode volume decreases the atom-field coupling, however, the collective coupling, which scales with the atom number, can remain large. At first, three groups started to set up experiments for studying collective effects in optical resonators. Vuletić at the MIT succeeded in trapping a few thousand atoms inside a confocal multimode cavity. In Tübingen and in Hamburg, Zimmermann [71] and Hemmerich [72] held nearly $10^6$ atoms inside a ring cavity, which has two counter-propagating degenerate modes.

The prospects for the collective cooling and trapping of a dilute atomic cloud in the field of an optical cavity were investigated theoretically for the first time by the Ritsch group in Innsbruck [73, 74]. In 2002, the numerical simulation of the transversely pumped system showed that for properly chosen parameters the atoms arranged into a regular pattern which supported effective cooling [75]. The initially homogeneous atom cloud illuminated from the side evolved – by spontaneous symmetry breaking – into one of the two possible lattices which scatter maximum field into the cavity via Bragg scattering.
The phenomenon is in close analogy with Dicke superradiance [76]. Two phases of the cavity field, differing by \( \pi \), correspond to the two possible atomic patterns. Within a year, this so-called self-organization phenomenon was demonstrated experimentally by Vuletić [77]. Further theoretical advance revealed that this was a real phase transition in the thermodynamic limit, where it could be well described by a mean-field model [78].

In a ring cavity, the self-organization is closely related to the collective atomic recoil lasing (CARL) [79, 80, 81], which originally introduced as a gain process analogous to the free electron laser [82]. In the Hamburg and Tübingen experiments [83, 84], one propagating mode of the ring cavity is driven, and above a pumping threshold, a stationary field builds up in the other mode along with the formation of a regular density pattern. Hence, the non-pumped mode is fed by coherent photon scattering on the atomic grating from the pumped mode. In 2007, the CARL process was demonstrated with both ultracold and Bose-Einstein condensed atoms [85].

More recently, a peculiar atom–cavity system has been realized [86]. At the ETH in Zurich, the Esslinger group succeeded in trapping a Bose-Einstein condensate of \( 10^5 \) Rb atoms inside an ultra-high finesse optical microcavity. Working in the far-detuned limit, they attained strong dispersive coupling between the atoms and the field. Even a single atom of the condensate realizes strong coupling to the field, hence the collective coupling of so many atoms is enormous. On the one hand, this means that the cavity is highly sensitive to the dynamics of the BEC, so for instance it can be used as a stroboscope to monitor matter-wave motion [87]. On the other hand, the field creates both coherent and incoherent excitations in the BEC. The cavity-mediated long-range atom–atom interaction has significant effects as it is in the same order of magnitude or even larger than the collisional interaction between the atoms. This exotic quantum many-body system shows a number of generic, collective effects [88, 89, 90], which are still being explored both by theory and by experiment.

### 1.4 Outline of the Thesis

The central part of this Thesis is devoted to the theoretical description of many-body effects occurring in a cloud of cold or ultracold atoms which is dispersively coupled to a high-finesse optical cavity. I describe the coupled atom–field dynamics on different levels, starting from a classical mean-field model through a mean-field Bogoliubov theory up to a full quantum simulation of the system in terms of a quantum master equation. In addition, at the end of the Thesis, I include a calculation on the induced dipole-dipole
interaction between the atoms. Generally this has a negligible effect, however, for strong laser fields it can eventuate the collapse of a dense atomic cloud.

Being more specific, in Chapter 2 of the Thesis, I review the basic theoretical tools for describing the atom–field interaction in optical cavities [63], thus providing a solid basis for the forthcoming chapters.

Chapter 3 deals with the cavity-induced self-organization in two different systems. In the first one, a thermal atomic cloud is coupled to the field of a ring resonator [91], while in the second one, a BEC interacts with a single-mode cavity [92]. Although a thermal cloud of atoms seems to be rather different from a BEC, the phase transition takes place similarly, since it arises from the same type of atom–field coupling. For both systems, I discuss the phenomenon in terms of a mean-field approach, and I draw a phase diagram as functions of the control parameters. In case of a BEC, the Bogoliubov excitation spectrum of the compound atom–cavity system is also calculated, which provides additional insight into the phase transition.

In Chapter 4 of this Thesis, I compute the excess noise depletion of a Bose-Einstein condensate arising from the interaction with the cavity field [93]. Even a zero-temperature BEC cannot fully occupy its ground state, since the atom–atom interactions kick out atoms to the excitation modes. In an optical cavity, besides the s-wave collisions the field-mediated atom–atom interaction together with the photon loss noise is a new source of depletion. I use Langevin equations linearized around the mean-field solution to calculate the steady-state atom number in the excited states of the condensate. The study of the depletion completes the mean-field model of Chapter 3, as it describes the error of the mean-field approximation.

In Chapter 5, I provide a full quantum simulation for a single-mode excitation of a BEC by a high-finesse optical cavity mode [94]. This system is formally analogous to a broad class of optomechanical systems, where micromechanical oscillators are coupled to resonator modes via the radiation pressure force. For weak fields, the cavity mode dominantly couples a homogeneous condensate to a single excitation mode (playing the role of the oscillator), onto which the dynamics can be restricted. By adiabatically eliminating the photon field, I derive a quantum master equation for this BEC excitation mode, which accounts for both the coherent and the dissipative parts of the dynamics due to the coupling of a driven, lossy mode of a resonator. Numerical simulation of our model allows for exploring the quantum limit of optomechanical systems in a classically bistable regime, and leads to better understanding the quantum back-action of the cavity field on the condensate in the experiments performed in Zurich [87, 95].
In Chapter 6 of this Thesis, I calculate the effect of the induced dipole-dipole interaction on the far-off-resonance trapping of cold atoms [96]. The laser field induces an atomic polarization which gives rise to a radiative atom–atom interaction that is disregarded in most cases. Nevertheless, at high densities and strong fields it can provoke the collapse of the cloud. I apply a mean-field approach to calculate the boundary of the stable equilibrium region, where the thermal motion of atoms stabilizes the gas against self-contraction. I draw a phase diagram, and discuss the limitations imposed by the dipole-dipole instability on the parameters needed to reach Bose-Einstein condensation in an optical dipole trap.

Finally, I summarize my results achieved during my Ph.D. in Chapter 7.
Chapter 2

Theoretical background

The aim of this chapter is to provide a general framework for the description of dispersive interaction between an atomic ensemble and the field of a high-finesse optical resonator, that constitutes a common basis for the collective phenomena discussed in this Thesis. Starting with the understanding of the atom–cavity interaction for a single atom and a single cavity mode, we introduce the standard approximations which lead to dispersive coupling. Then, we outline the construction of the mean-field models both for a thermal atomic cloud and for a Bose-Einstein condensate.

2.1 Single atom motion inside a single mode cavity

Atoms are characterised by external (motional, i.e. position and momentum) and internal (electronic) degrees of freedom. They interact with the electromagnetic field via their transition dipole moment, meaning that light couples different electronic states of the atoms. However, in the optical domain the atomic motional states are also coupled by the photon scattering process. In the beginning, we are going to deal with the internal dynamics of the atom in which its external position appears as a parameter. Then, we release the atom and derive the light forces defining its motion. The dissipative atom–cavity dynamics can be described by two equivalent approaches, either by a master equation for the reduced density operator of the system, or by the Heisenberg–Langevin equations which include noise terms to account for dissipation. We use both approaches in this Thesis, always the one which fits the given problem best. Finally, we eliminate the excited atomic level and explain why spontaneous emission can be neglected in the far-detuned limit.
2.1.1 Jaynes–Cummings model

We begin with the description of the dipole coupling between a single atom and a single quantized mode of the electromagnetic field. Let us consider two energy levels of the atom, separated by $\hbar \omega_A$. The corresponding atomic states constitute an orthonormal basis of a closed two-dimensional Hilbert space. The ground state $|g\rangle$ is assumed to be stable, while the excited state $|e\rangle$ is allowed to spontaneously decay to the ground state. It is convenient to describe this so-called two-level atom by associating a spin-half to it. Thus, we can use the Pauli spin operators,

$$
\sigma = |g\rangle \langle e|,
$$

$$
\sigma^\dagger = |e\rangle \langle g|,
$$

$$
\sigma_z = \frac{1}{2} (|e\rangle \langle e| - |g\rangle \langle g|),
$$

which fulfill the commutation relations of the spin-half operator algebra. The first two of them are the atomic lowering and raising operators, whilst the third one is the atomic inversion operator. The Hamilton operator of the atom then becomes

$$
H_A = \hbar \omega_A \langle e| e\rangle = \hbar \omega_A \sigma^\dagger \sigma = \hbar \omega_A \left( \sigma_z + \frac{1}{2} \right).
$$

Since the electron wave functions in the stationary states are centrosymmetric, the $2 \times 2$ matrix of the dipole moment operator $\hat{d} = e \hat{r}$, has zero diagonal elements, moreover its off-diagonal elements become the same real vector $\hat{d}$ for a properly chosen global phase. Consequently, the atom has a transitional dipole moment which corresponds to electronic transitions, and can be expressed with the spin operators as

$$
\hat{d} = d (\sigma + \sigma^\dagger),
$$

with the sole off-diagonal matrix element $d = d_{eg} = d_{ge} = \langle g| \hat{d}|e\rangle$.

The electric field operator of a quantized electromagnetic field mode of frequency $\omega$ is given in the Schrödinger picture by

$$
\hat{E}(r) = i \sqrt{\frac{\hbar \omega}{2 e_0 V}} e^{i(f(r)a - f^*(r)a^\dagger)},
$$

where $f(r)$ is the mode function, $e$ is the polarization vector, and $V$ is the mode volume. The operators $a^\dagger$ and $a$ are the photon creation and annihilation operators. By considering, for instance, the single TEM00 mode of a high-$Q$ optical resonator, its mode function can be simply taken $f(x) = \cos k x$ along the direction of the cavity axis $\hat{x}$, with
the wavenumber $k = 2\pi/\lambda$. In the transverse direction it has a Gaussian shape determined by the cavity waist. The expression Eq. (2.4) reveals the scaling of the electric field with the mode volume. While in free space $V$ is a fictitious quantization volume, in a cavity, it is given by a well-defined Gaussian mode between the mirrors; $V = \int |f(r)|^2 d^3r$, where $\text{sup}\{|f(r)|\} = 1$. Hence, the field of a single photon becomes larger as the cavity mode volume is decreased. The Hamilton operator of a quantized cavity mode is simply $H_C = \hbar \omega_C a^\dagger a$, with $\omega_C$ being the frequency of the cavity resonance.

The atom–field interaction can be treated within the dipole approximation. As the atomic radius is much smaller than the optical wavelengths, the spatial variation of the electric field is neglected on the atomic length scale. The atom is regarded as a pointlike dipole which interacts with the electric field at its actual position $r$. In this spirit, the interaction Hamiltonian is written as

$$H_{AC} = -\hat{d}\hat{E}(r) = -i\sqrt{\frac{\hbar \omega}{2\epsilon_0 V}} \nabla (\sigma + \sigma^\dagger)(f(r)a - f^*(r)a^\dagger). \quad (2.5)$$

When the energy scale of the interaction is dwarfed by the atomic and photonic excitation energies, only those terms play important role in the dynamics, which conserve the excitation number. Therefore, in the rotating wave approximation, we neglect the terms containing two creation or two annihilation operators, which are counter-rotating in the Heisenberg picture, arriving to the Jaynes-Cummings model [97],

$$H'_{JC} = \hbar \omega_C a^\dagger a + \hbar \omega_A \sigma_z - i\hbar g(r)(\sigma^\dagger a - a^\dagger \sigma). \quad (2.6)$$

Here, we assumed a real mode function and introduced the single photon Rabi frequency describing atom-photon coupling, $g(r) = g_0 f(r)$, with the maximum value $g_0 = \sqrt{\frac{\omega_C}{2\epsilon_0 V}} \nabla$. Finally, we transform the above Hamilton operator into a frame rotating with the driving frequency $\omega$ that corresponds to the laser excitation. As a result, two relevant frequency parameters appear in our model, the atomic detuning $\Delta_A = \omega - \omega_A$ and the cavity detuning $\Delta_C = \omega - \omega_C$. The transformation of the operators is straightforward, hence we keep their original notation, however, the detunings refer to the rotating frame. The transformed Hamilton operator then reads

$$H_{JC} = -\hbar \Delta_C a^\dagger a - \hbar \Delta_A \sigma_z - i\hbar g(r)(\sigma^\dagger a - a^\dagger \sigma). \quad (2.7)$$

Because of the rotating wave approximation, the Jaynes-Cummings Hamilton operator preserves the number of excitation quanta in the system. Consequently, the states with a fixed $(n+1)$ excitation number form an invariant subspace spanned by the basis vectors $|e, n\rangle$ and $|g, n+1\rangle$. The eigenstates of the system are usually referred to as
“dressed states”, and they are easily obtained by the rotation of these two basis vectors. Note that the atom-field coupling \( g(\mathbf{r}) \) depends on the atomic position \( \mathbf{r} \). Thus, if the atom being initially in its ground state enters into interaction with the field, the system remains in the same eigenstate, which adiabatically follows the slow atomic motion. The energy of the corresponding dressed state signifies a real optical potential for the atomic central mass motion. Depending on the sign of the detunings, a ground state atom can feel potential hills or valleys at the intensity maxima of the field.

### 2.1.2 Quantum master equation

Hitherto we have discussed the coherent dynamics of an atom and a cavity mode. Nevertheless, both of them interact with the environment which is constituted by the vacuum field modes. As a result excitations of the system decay via two possible dissipation channels, namely, by spontaneous emission from the excited atomic level or by leaking out of cavity photons through the mirrors. These processes are characterized by the atomic spontaneous emission rate \( 2\gamma \) and the photon loss rate of the cavity denoted by \( 2\kappa \). The continuum of vacuum modes forms a broadband reservoir, whose correlation functions decay on a much shorter time scale than that of the relevant dynamics of the system. This allows one to invoke the Markov approximation, which assumes that the fluctuations in the reservoir are \( \delta \)-correlated, hence their back-action on the system is a white noise. Accordingly, the environment has no memory in the sense that information entering it does not come back. In other words, the Markov approximation separates the system (atom plus cavity) from the environment (vacuum modes) by slaving the environment variables to the system variables.

The standard formalism which describes the dissipative dynamics of open quantum systems relies on an equation of motion for the reduced density operator \( \rho \), that is given by tracing out the environmental degrees of freedom from the density operator of the closed grand system containing the environment [98]. This quantum master equation takes the following general form

\[
\dot{\rho} = \frac{1}{i\hbar} [H, \rho] + \mathcal{L}\rho, \tag{2.8}
\]

where the Hamilton operator \( H \) and the Liouvillian superoperator \( \mathcal{L} \) describe the conservative and the dissipative parts of the dynamics, respectively. In fact, the Neumann equation for the density operator is amended by terms that take into account environmental effects resulting in decay and diffusion.
Figure 2.1: Scheme of a linear resonator showing the pumping and loss processes.

For simplicity, we present the master equation for a single atom interacting with a single cavity mode, that can be generalized for more atoms and modes by a straightforward summation. We allow for both pumping methods applied in the experiments (see Fig. 2.1): the direct feeding of the cavity mode via one of the mirrors (described by the parameter \( \eta \)) and the transverse pumping scheme, where the atom is illuminated from the side by a laser standing wave (whose strength is measured by the Rabi frequency \( \Omega \) of the atom). We assume that the two pumps have the same frequency and the same phase.

Our model Hamiltonian for the atom–cavity system then reads

\[
H = \frac{p^2}{2m} - \hbar \Delta_A \sigma_z - \hbar \Delta_c a^\dagger a - i \hbar g(r) \left( \sigma^\dagger a - a^\dagger \sigma \right) \\
- i \hbar \eta (a - a^\dagger) - i \hbar \Omega(r) \left( \sigma^\dagger - \sigma \right). \tag{2.9}
\]

The first line is the Jaynes-Cummings Hamiltonian, Eq. (2.7) complemented by the kinetic energy of the atom, while the second line contains the cavity and the atomic pumping terms. The atom–field interaction term and the atomic pump term depend on the position of the atom through the cavity mode function as \( g(r) = g_0 f(r) \), and through the spatial variation of the transverse pumping field as \( \Omega(r) = \Omega h(r) \), respectively. These terms couple the atomic motional degrees of freedom.

The Liouvillian superoperator is given by

\[
\mathcal{L}_\rho = \kappa \left( 2 a \rho a^\dagger - \{a^\dagger a, \rho\} \right) + \gamma \left( 2 \int d^2u \ N(u) \sigma e^{-ik_A ur} \rho e^{ik_A ur} \sigma^\dagger - \{\sigma^\dagger \sigma, \rho\} \right). \tag{2.10}
\]

Here the first term describes the cavity decay, and the second term stands for the atomic spontaneous emission. The notation \( \{\ , \} \) is used for the anticommutator. The
atom of mass $m$ has position $\mathbf{r}$ and momentum $\mathbf{p}$ fulfilling $[r_\alpha, p_\beta] = i\hbar \delta_{\alpha\beta}$. In the second term, there is an averaging over the random direction (denoted by the unit vector $\mathbf{u}$) of the spontaneously emitted photon with the direction distribution $N(\mathbf{u})$ characteristic to the given atomic transition. The wavenumber $k_A$ corresponds to the atomic transition frequency $\omega_A$. Note that the wavenumbers in our system are practically all equal, since the detunings are much smaller than the optical frequencies themselves: $\Delta_A, \Delta_C \ll \omega, \omega_A, \omega_C$, therefore $k_A \approx k_C \approx k$.

### 2.1.3 Heisenberg–Langevin equations and bosonization

The internal dynamics of the atom defined by the Hamiltonian (2.9) and the Liouvillean (2.10) is the source of a wealth of interesting phenomena that are widely studied in quantum optics, such as Rabi oscillations and atom–field entanglement [99]. Nevertheless, we focus on the external atomic dynamics, therefore we shall simplify the presented model by eliminating the atomic internal degrees of freedom. To do this, we use a description that is equivalent to the master equation, namely the Heisenberg-Langevin equations for the system operators.

As a starting point, we adiabatically separate the timescales of the atomic internal and external motions. We assume the that the atom is moving slowly in the field such that the the corresponding frequency is much smaller than the decay rates of the internal dynamics, expressed for the velocity, $kv \ll \kappa, \gamma$. This means, on the one hand, that the atomic polarization relaxes to its steady state value defined by the field at the current atomic position. On the other hand, the external degrees of freedom become just parameters for the internal dynamics.

In the Heisenberg picture, the equations of motion of the atomic and the field operators are given by their commutators with the Hamilton operator. In case of dissipation, however, correlated noise operators together with decay terms appear in the equations of motion, in agreement with the fluctuation-dissipation theorem. They arise from the interaction of the system with the vacuum field. The expectation values of the Langevin noise operators are zero, whereas their correlations describe diffusion. The Heisenberg-Langevin equations are derived via the elimination of the vacuum modes by formally integrating their equations of motion in the Heisenberg picture, and using the Markov approximation (see page 394 of Ref. [100]). Such a description of the system is equivalent to the one provided by the master equation for the reduced density operator Eq. (2.8). Nevertheless, it is more suitable for certain problems, e.g. for the adiabatic elimination
of the atomic polarization.

The Heisenberg-Langevin equations for the field and the atomic internal variables then read

\[ \dot{a} = (i\Delta_C - \kappa)a + Ng^*(r)\sigma + \eta + \xi, \]
\[ \dot{\sigma} = (i\Delta_A - \gamma)\sigma + 2g(r)\sigma_z a + 2\Omega(r)\sigma_z + \zeta, \]
\[ \dot{\sigma}_z = -g(r)(\sigma^\dagger a + a^\dagger \sigma) - \Omega(r)(\sigma^\dagger + \sigma) - \gamma(\sigma_z + 1/2) + \zeta. \]

The non-zero two-time correlation functions of the Langevin noise operators are

\[ \langle \xi(t_1)\xi^\dagger(t_2) \rangle = 2\kappa\delta(t_1 - t_2), \]
\[ \langle \zeta(t_1)\zeta^\dagger(t_2) \rangle = 2\gamma\delta(t_1 - t_2), \]
\[ \langle \zeta_z(t_1)\zeta^\dagger_z(t_2) \rangle = 2\gamma\langle \sigma^\dagger \rangle\delta(t_1 - t_2), \]
\[ \langle \zeta(t_1)\zeta_z(t_2) \rangle = 2\gamma\langle \sigma \rangle\delta_{kl}\delta(t_1 - t_2), \]
\[ \langle \zeta_z(t_1)\zeta_z(t_2) \rangle = 2\gamma(\langle \sigma_z \rangle + 1/2)\delta(t_1 - t_2). \]

In equations (2.11), the electromagnetic field is also a variable – in contrast to free-space laser cooling – that leads to a coupled nonlinear atom-field dynamics. For large atom-pump detuning, when the atomic saturation remains small, one can replace the inversion operator \( \sigma_z \) with its expectation value in the ground state, thus \( 2\langle \sigma_z \rangle \approx -1 \).

This approximation is called bosonization of the atomic dipole, since the atomic operators then satisfy the bosonic commutation relation \( [\sigma, \sigma^\dagger] = -2\sigma_z \approx 1 \). As we neglect the dynamics of the \( \sigma_z \) operator, we also set \( \zeta_z \) to zero. The bosonization, hence, linearizes the remaining Heisenberg-Langevin equations (2.11a,b), by breaking the atom-field correlation \( \langle \sigma^z a \rangle = -1/2\langle a \rangle \). Interestingly, this relation is exactly valid when there is only one excitation quantum in the system [101].

### 2.1.4 Linearly polarizable particle and the dispersive limit

In the large atomic detuning limit (when \( |\Delta_A| \) far exceeds the other parameters \( g_0\langle a \rangle, \Omega, k\nu \)), the internal dynamics follows the external atomic motion in the radiation field, hence the atomic operators \( \sigma, \sigma^\dagger \) can be adiabatically eliminated from the model. This simplifies the atom to a linearly polarizable particle. This could seem a severe restriction, however, it also constitutes a generalization of our model in the sense that it will apply to a general class of polarizable particles, e.g. to molecules.
Technically, one averages out the fast oscillation of the atomic operator $\sigma$ with $\Delta_A$ on an intermediate time scale $\delta t$ such that $\delta t \gg \Delta_A^{-1}$, but $\delta t$ remains still small on the time scale of the relevant dynamics. Formally, this is equivalent to the $\sigma$ operator expressed from Eq. (2.11b) by setting the left hand side $\dot{\sigma} = 0$. Introducing the operator of the dimensionless electric field

$$\hat{E}(r) = f(r)a + \Omega(r)/g_0,$$  \hfill (2.13)

the atomic polarization operator then becomes

$$\sigma \approx \frac{g}{i\Delta_A - \gamma} \hat{E}(\hat{r}) = -\frac{1}{g}(iU_0 + \Gamma_0) \hat{E}(\hat{r}),$$  \hfill (2.14)

where

$$U_0 = \frac{g_0^2\Delta_A}{\Delta_A^2 + \gamma^2}, \quad \Gamma_0 = \frac{g_0^2\gamma}{\Delta_A^2 + \gamma^2}. $$  \hfill (2.15)

Physically, the parameters $U_0$ and $\Gamma_0$ correspond to the real and imaginary parts of the complex susceptibility $\chi$ of the atom, since they describe the linear relationship between the atomic polarization and the electric field according to $P = \epsilon_0 \chi E$. With the usage of Eq. (2.3) and Eq. (2.14), $U_0$ and $\Gamma_0$ are expressed with the susceptibility $\chi = \chi' - i\chi''$ by

$$U_0 = -\frac{\omega_C}{V} \chi', \quad \Gamma_0 = -\frac{\omega_C}{V} \chi'',$$  \hfill (2.16)

where $\omega_C$ is the mode frequency and $V$ is the mode volume.

Inserting the above approximation Eq. (2.14) of the atomic operators into the original Hamilton operator (2.9), we get the following effective Hamiltonian

$$H_{\text{eff}} = \frac{p^2}{2m} - \hbar \Delta_C a^\dagger a - i\hbar\gamma(a - a^\dagger) + \hbar U_0 \hat{E}(r) \hat{E}(r).$$  \hfill (2.17)

Here the last term can be expanded as

$$\hbar U_0 f^2(r)a^\dagger a + \hbar\gamma f(r) h(r)(a + a^\dagger) + \hbar U_0 \frac{\Omega^2}{g_0^2} h^2(r).$$  \hfill (2.18)

The effective Liouvillian arising from the adiabatic elimination is

$$L_{\text{eff}} \rho = \kappa \left( 2a a^\dagger \{-a^\dagger a, \rho\}_+ \right) - \Gamma_0 \{E^\dagger(\hat{r}) E(\hat{r}), \rho\}_+$$
$$+ 2\Gamma_0 \int d^3u \ N(u) \hat{E}(\hat{r}) e^{-ik_A u} \rho e^{ik_A u} E^\dagger(\hat{r}).$$  \hfill (2.19)

These effective operators describe the coupled dynamics of the external motion of the linearly polarizable particle and the cavity field according to the quantum master equation (2.8). The field creates an optical potential for the atom that is proportional to $U_0$, and conversely, the atom sitting at a field maximum shifts the cavity resonance frequency
by $U_0$ and causes an effective cavity decay with rate $\Gamma_0$. On a microscopic level, the former and the latter effects can be connected with the atomic induced and spontaneous emission processes. Furthermore, the atomic pump $\Omega$ gives rise to an effective pumping strength for the cavity mode that is $\eta_\ell = \Omega g_0 \Delta_A/(\Delta_A^2 + \gamma^2)$. It arises from the coherent scattering of photons from the transverse pump into the cavity, hence it depends on the atomic position along the cavity axis $\hat{x}$ via the cavity mode function as $\eta_\ell(x) = \eta_\ell f(x)$.

Now, we are prepared to consider the \textit{dispersive limit} of the atom–cavity interaction. This is the same limit that is taken in the far-off-resonance trapping scheme [10], and it also applies to CQED [67]. It is seen from Eq. (2.15) that $U_0$ and $\Gamma_0$ scale differently with the atomic detuning $\Delta_A$. Namely, for large $\Delta_A$, $U_0 \approx g_0^2/\Delta_A$, while $\Gamma_0 \approx g_0^2 \gamma/\Delta_A^2$. Thus, their ratio $\Gamma_0/U_0 \approx \gamma/\Delta_A$ tends to zero as $\Delta_A$ increases. The depth of the optical potential, however, is given by $U_0(a^\dagger a)$. Therefore, one can suppress spontaneous emission while keeping the optical forces on a constant level by increasing the atomic detuning $\Delta_A$ together with either of the pumping strengths $\eta$ or $\eta_\ell$. In the experiments, $|\Delta_A|$ can easily be tuned up to 100...1000$\gamma$ at reasonable laser powers. In the dispersive limit, we neglect the effects stemming from atomic spontaneous emission, and set $\gamma = 0$, $\Gamma_0 = 0$. With this, we erase the last two terms of the effective Liouvillian operator Eq. (2.19), saying that dissipation of the system is only possible via the cavity field mode.

### 2.2 Mean-field theory

Up to this point, we have discussed the coupled dynamics of a single atom and a single cavity mode. The motion of a single atom inside a cavity is an appealing system producing effects such as dynamical cavity cooling [60]. The correlated motion of a few atoms interacting with the cavity field is also an interesting problem resulting in cavity mediated cross friction [102] and motional entanglement [103, 104]. In this Thesis, however, we are interested in collective effects produced by a large number of atoms. So as to describe such a system, we need to make further approximations regarding the atomic external degrees of freedom.

One possibility is the \textit{semiclassical approximation}, which assumes that the atomic wave packets are well localized in both position and momentum spaces [4]. Hence, one can describe the external atomic motion with classical variables, obeying the classical Langevin equations derived from the operator equations of motion [63]. Using this approximation, one can simulate the dynamics of a cold atomic ensemble coupled to a single cavity mode for up to a few thousand atoms [78].
The other possibility is the mean-field approach, which reduces the many-body problem to an effective one-body problem by assuming that all atoms move in the same mean-field potential created by the field of the cavity. This also includes the assumption that the field, reaching its steady-state on a faster time scale, adiabatically follows the atomic motion. Thus, we exclude effects like cavity cooling which are based on the delayed dynamics of the field. In the mean-field model, the cavity field is determined solely by atomic ensemble averages, thus the back-action of each individual atom is neglected. An important advantage of this approach is that it corresponds to the thermodynamic limit of the system, where the atom number $N \rightarrow \infty$, the single atom coupling $g_0 \rightarrow 0$, while the collective coupling described by $N g_0^2$ or $NU_0$ is kept constant. In a physical realization of the limit, the cavity volume would be increased (by raising the cavity length $l_{\text{cav}}$) at a constant atomic density, which would decrease the coupling according to $g \propto 1/\sqrt{N}$. Since the photon round trip time increases with the cavity length, the reflexivity of the mirrors has to scale as $\propto 1/l_{\text{cav}}$ to keep $\kappa$ constant.

The mean-field model can be thought of as a self-consistent field theory. The density distribution of the atoms simultaneously fixes the steady state of the cavity mode (which is a coherent state), and the corresponding optical potential acts back on the atomic distribution. Hence, the mean-field solution has to be determined self-consistently. In practice, we calculate it by the numerical iteration of the atomic density with the self-consistent potential.

In Chapter 3 the Reader will see, that the mean-field description gives qualitatively similar results both for a thermal cloud and a Bose-Einstein condensate of the atoms. This is so, because the cavity field depends exclusively on the atomic density distribution, hence it provides the same optical potential for a given distribution irrespective of the motional quantum states of the atoms.

Fluctuations are absent in the mean-field model, however, they may be taken into account by expanding the original equations of motion of the system around the mean field. In this context, the mean-field theory can be regarded as the zeroth-order expansion of the problem in the fluctuations. In this Thesis we are dealing with the self-consistent mean-field solution, and the first-order fluctuations around it. In the studied systems, fluctuations play an important role because of two reasons. First, they induce a phase transition of the atomic cloud placed inside the resonator from a homogeneous to a periodically modulated phase. This so-called self-organization is investigated in detail in Chapter 3. Second, in the case of a BEC, certain matter wave fluctuations are driven by the quantum noise of the cavity field. In Chapter 4, we calculate the steady-state
population in these excited motional states which measures the depletion of the atoms from the condensate. Finally, in Chapter 5, we specifically deal with the dynamics of a given condensate excitation mode around a trivial (constant) mean-field solution.

2.2.1 Mean-field model for thermal atoms

For the description of a cold atomic sample, we can safely use both the semiclassical and the mean-field approximations. Accordingly, the atomic external variables are treated classically, and the cloud is characterized by a continuous density distribution $p(x)$, when considering the atomic motion in one dimension along the cavity axis $\hat{x}$.

In order to get a self-consistent mean-field theory for the atoms in the thermodynamic limit, we phenomenologically add the assumption that the cloud has a finite temperature $T$. Then, we can apply the canonical distribution to the gas, which reads

$$p(x) = \frac{1}{Z} \exp \left( -\frac{V(x)}{k_B T} \right),$$

with the partition function $Z$ ensuring normalization $\int p(x) dx = 1$. The mean-field potential $V(x)$ is derived from the effective Hamiltonian (2.17) by substituting the steady-state coherent amplitude of the cavity field $\alpha$ for the operator $a$,

$$V(x) = \hbar U_0 f^2(x)|\alpha|^2 + \hbar \eta f(x)(\alpha + \alpha^*).$$

Note that $\alpha$ depends on the distribution $p(x)$ itself. Since the field is assumed to adiabatically follow the motion of the atoms, it can be determined as the steady-state of the master equation defined by the many-body version of the effective Hamilton and Liouville operators Eqs. (2.17,2.19) for frozen atomic dynamics. As follows $\alpha$ is expressed by

$$\alpha = \frac{\eta - iN\eta \langle f(x) \rangle}{\kappa - i(\Delta_C - NU_0(f^2(x)))},$$

where $U_0$ is the one-atom light shift, $\eta$ is the effective transverse pumping strength in the dispersive limit and $N$ is the atom number. The average $\langle \ldots \rangle$ is taken over the atomic distribution, like $\langle f(x) \rangle = \int f(x)p(x) dx$.

We find numerical solutions to the implicit equation (2.20) by iterating the following steps. (i) Start from a random distribution $p^{(0)}(x) = \lambda^{-1} + \xi(x)$, where $\xi(x)$ is a white noise: $\langle \xi(x)\xi(x') \rangle = \epsilon \delta(x - x')$, with amplitude $\epsilon \ll \lambda^{-2}$. (ii) Obtain from (2.22) the steady-state mode amplitude $\alpha$ for the given distribution $p^{(0)}(x)$. (iii) Calculate the dipole potential $V(x)$ by substituting $\alpha$ into (2.21). (iv) The canonical distribution eq. (2.20)
furnishes the new distribution \( p^{(1)}(x) \) with which the procedure can be restarted. If the iteration converges, we obtain a self-consistent solution of (2.20), \( p(x) = p^{(\infty)}(x) \).

The presented mean-field model constitutes an effective tool to describe cold atoms in general, with the potential \( V(x, p(x)) \) chosen for the given problem. Microscopic calculations reveal that the canonical distribution is indeed a good approximation for an atomic ensemble inside the resonator [62], furthermore the temperature is on the order of \( k_B T \approx \hbar \kappa \) in case of cavity cooling [60]. In the first part of Chapter 3, we apply this model to a ring resonator which has two degenerate counterpropagating modes, therefore the mean-field potential takes a more complex form. The model is also suitable to take into account the induced dipole-dipole interaction between the atoms, which we calculate in Chapter 5 of this Thesis.

### 2.2.2 Mean-field theory for a BEC

The semiclassical approximation fails to describe situations where the quantum motion of the atoms is relevant, e.g. in case of ultracold atoms, or when ground state cooling [105] is reached. Nevertheless, the direct solution of the quantum many-particle problem including the external motion is practically impossible, therefore one has to simplify the system. From a theoretical point of view, probably the simplest form of an ultracold quantum gas is the Bose-Einstein condensate (BEC), because it can be well described in terms of a mean-field theory. Indeed, most of its atoms (typically more than 95 \%) are sitting in the ground state of the corresponding mean-field potential, because the atom-atom interactions are relatively small. This validates the Gross-Pitaevskii equation which describes the dynamics of a single condensate wave function. A useful tool supplementing the mean-field description is the Bogoliubov approach which considers small fluctuations around the mean-field solution in linear order. For a detailed discussion, consult Ref. [106].

In the dispersive limit, we construct the many-particle version of the effective Hamiltonian (2.17) in one dimension, which contains the atomic field operator \( \Psi(x) \),

\[
H = -\hbar \Delta_C \alpha^1 - i \hbar \eta (a - a^\dagger) + \int \Psi(x) \left[ -\hbar^2 \frac{d^2}{dx^2} + \frac{g}{2} \Psi(x) \Psi(x) \right] dx \\
+ \int \Psi(x) \left[ \hbar U_0 f^2(a^\dagger a + \hbar \eta f(x)(a + a^\dagger)) \right] \Psi(x) dx.
\]

The first line gives the free evolution of the resonator mode and the atom field, whereas the second line accounts for the dispersive interaction between them. Compared to Eq. (2.17), a new fourth order term appears at the end of the first line, which takes into
account s-wave collisions [106]. Its strength is given by the s-wave scattering constant \( g_c \), that is proportional to the s-wave scattering length \( a \) according to \( g_c = 4\pi\hbar a/(mw^2) \), and also depends on the transverse size \( w \) of the condensate in one dimension.

The equations of motion of the field operators \( a \) and \( \Psi \) in the Heisenberg picture become

\[
\frac{i}{\hbar} \frac{d}{dt} a = \left[ -\Delta + \int \Psi^\dagger (x,t) \Psi(x,t) U(x) \, dx - i\kappa \right] a \\
+ \int \Psi^\dagger (x,t) \Psi(x,t) \eta(x) \, dx + i\eta + i\xi, \quad (2.24a)
\]

\[
\frac{i\hbar}{\partial t} \Psi(x,t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \hbar a^\dagger a U(x) \right. \\
+ \hbar \eta(x)(a + a^\dagger) + g_c \Psi^\dagger (x,t) \Psi(x,t) \right] \Psi(x,t). \quad (2.24b)
\]

Here, we use the notations \( U(x) = U_0 f^2(x) \) and \( \eta(x) = \eta f(x) \). The noise operator \( \xi \) is the same as in Eq. (2.11a), and its correlation is given by Eq. (2.12a). Similarly to the single atom case, the atomic cloud shifts the frequency of the mode and yields an effective transverse pump for the cavity, and these effects are proportional to the atomic density operator \( \Psi^\dagger (x,t) \Psi(x,t) \). Generally speaking, Eqs. (24) provide the description of dispersively coupled matter and radiation fields.

Now, we turn to the mean-field model which is the most convenient way to describe a Bose-Einstein condensate. The basic idea is that one separates the operators to a mean value and to fluctuations around it,

\[
a(t) = \alpha(t) + \delta a(t), \quad (2.25a)
\]

\[
\Psi(x,t) = \sqrt{N}\psi(x,t) + \delta \Psi(x,t). \quad (2.25b)
\]

For the cavity mode, the mean value \( \alpha \) is the complex amplitude of the coherent state \( |\alpha(t)\rangle \), given by \( \alpha(t) = \langle a(t) \rangle \). Similarly, for the atom field \( \psi(x,t) = N^{-\frac{1}{2}} \langle \Psi(x,t) \rangle \) is the so-called condensate wave function, that is normalized to unity. As a consequence of the above definition, the fluctuations have zero mean. Substituting the means for the operators in Eqs. (2.24), one obtains their coupled Gross-Pitaevskii-like equations of motion,

\[
\frac{i}{\hbar} \frac{d}{dt} \alpha(t) = \left[ -\Delta + N \langle U(x) \rangle - i\kappa \right] \alpha(t) + i\eta + \langle \eta(x) \rangle, \quad (2.26a)
\]

\[
\frac{i\hbar}{\partial t} \psi(x,t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \hbar |\alpha(t)|^2 U(x) \right. \\
+ \hbar (\alpha(t) + \alpha^\dagger(t)) \eta(x) + g_c N |\psi(x,t)|^2 \right] \psi(x,t), \quad (2.26b)
\]
where the averages are taken over the atomic distribution expressed with the condensate wave function, as \(\langle U(x) \rangle = \int |\psi(x, t)|^2 U(x) \, dx\).

As with the nondegenerate atom gas, the dynamics of the cavity field can be adiabatically eliminated from the system. For ultracold atoms, this approximation is far better than for a thermal cloud, since the atomic motion is slower. In fact, the photon loss rate \(\kappa\) is typically at least one order of magnitude higher than the recoil frequency \(\omega_R = \hbar k^2/(2m)\), which gives the scale of the atomic kinetic energy. From Eq. (2.26a), one obtains the same expression for the coherent field amplitude \(\alpha\) as the one in Eq. (2.22) derived for thermal atoms. The only difference is that the condensate wave function enters into the averages over the atomic distribution. Hence, one arrives at a Gross-Pitaevskii equation (GPE) for the condensate wave function,

\[
\frac{i\hbar}{\partial t} \psi(x, t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \hbar |\alpha|^2 U(x) + \hbar (\alpha + \alpha^*) \eta_k + g_c N |\psi(x, t)|^2 \right] \psi(x, t),
\]

with a mean-field optical potential that contains the steady-state cavity field amplitude \(\alpha\) defined in Eq. (2.22), which is in turn a function of \(\psi(x, t)\).

Compared to the mean-field model for a thermal cloud, here we do not have to assume an explicit form for the atomic distribution, instead we can solve directly the quantum motion of the atoms. We obtain the self-consistent solution of Eqs. (2.27,2.22) with the help of an imaginary-time propagation method. A stationary BEC state \(\psi(x)\) evolves according to

\[
\psi(x, t) = \psi(x) \exp^{-i\mu t/\hbar},
\]

where \(\mu\) is the energy of the stationary state (for the ground state in the mean-field approach, it amounts to the chemical potential). Starting from an arbitrary normalized wave function, we numerically propagate the GPE in imaginary time \(\tau = it\). All components of the initial wave function decay in imaginary time, but, the excitations of the condensate decay faster than the ground state, since their energy \((\mu)\) is larger. On the long run, any initial wave function converges to the ground state wave function, if they are not orthogonal to each other. (The solution is continuously renormalized after some propagation time). This method gives the ground state \(\psi_0(x)\), its energy \(\mu_0\) and the corresponding steady-state field amplitude \(\alpha_0\) with arbitrary precision.

The above discussed model forms the basis for the description of a BEC in an optical cavity. It is applied directly in the second part of Chapter 3, whereas it serves as a starting point for studying the spectrum, the incoherent excitation and the dynamics of the fluctuations around the mean-field solution in Chapter 3, 4 and 5, respectively.
Chapter 3

Mean-field model of self-organization

In this chapter, I present my results concerning the self-organization of an atom cloud due to the dispersive interaction with the field of a high quality optical resonator. I study the phenomenon for two different atomic ensembles and two cavity geometries. In Section 3.1, I consider a thermal atomic cloud inside a ring resonator, that has two degenerate counterpropagating field modes. Whereas, in Section 3.2, I deal with the self-organization of a Bose-Einstein condensate interacting with a single cavity mode. I describe the phenomenon within the framework of the mean-field model introduced in Section 2.2. Although the two systems are different, the mean-field model of self-organization establishes a common ground for them. From the field’s point of view, it is irrelevant whether there is a thermal cloud or a Bose-Einstein condensate inside the resonator. Furthermore, the Reader will see that even in a two-mode ring resonator it is only one cavity eigenmode which plays an important role in the phase transition. Hence, it is understood on a more general level when comparing the results obtained for different systems.

As outlined in the Introduction, the self-organization effect was first pointed out in Ref. [75] in 2002. Since then, considerable theoretical and experimental efforts were devoted to the understanding of the phenomenon [107]. The mean-field description for a thermal cloud in a single mode cavity was developed by Asbóth in Ref. [78], which provided a simple explanation in terms of adiabatic mean-field potentials. In this Chapter, after evoking the original model, I step forward in two directions. First, in Section 3.1, I generalize the model for the field of a ring cavity and discuss the results published in Ref. [91]. This work was motivated by the experiments performed with cold atoms inside a ring resonator [83, 84]. Second, in Section 3.2, I establish the mean-field model for a BEC, following the lines of Ref. [108], and present the results published in Ref. [92].
Coupling a BEC to the field of a high-finesse cavity is an interesting topic which has only recently come into experimental reach [85, 87].

We begin by recalling the explanation of self-organization in terms of the adiabatic mean-field potential created by the field of a single mode optical cavity [78]. In order to gain some physical insight, it is appropriate to adiabatically eliminate the cavity field as discussed in Section 2.2.1. The coherent amplitude of the field is given by Eq. (2.22), which gives rise to the optical potential of Eq. (2.21). For a cavity mode function $f(x) = \cos kx$, this self-consistent potential becomes

$$ V(x) = U_1 \cos kx + U_2 \cos^2 kx , $$

which is the sum of a $\lambda$ and a $\lambda/2$ periodic term. The coefficients are

$$ U_1 = 2 \langle \cos kx \rangle N I_0 \left[ \Delta_c - N U_0 \langle \cos^2 kx \rangle \right] , $$

$$ U_2 = \langle \cos kx \rangle^2 N^2 I_0 U_0 . $$

It is important to emphasize that the potential $V(x)$ has the same form for a thermal gas and for a BEC. For a thermal cloud, it shapes the canonical distribution Eq. (3.14), whereas for a condensate it appears in the Gross-Pitaevskii equation (2.27). The nonlinearity of the system is introduced by the dependence of the coefficients on the atomic distribution via the specific mean values

$$ \Theta = \langle \cos kx \rangle , $$

which can be considered as an order parameter, and

$$ B = \langle \cos^2 kx \rangle , $$

which is called the bunching parameter. The averages are calculated for the two ensembles either by $\langle \ldots \rangle = \int p(x) \ldots dx$, or by $\langle \ldots \rangle = \int |\psi_0(x)|^2 \ldots dx$. The order parameter $\Theta$ describes the $\lambda$-periodic spatial order of $\psi_0$: $\Theta = 0$ for a uniform distribution, and $\Theta = \pm 1$ for the atoms being localized around the ‘even’ ($kx = 2n\pi$), or ‘odd’ field antinodes ($kx = (2n+1)\pi$), respectively. The bunching parameter reflects the degree of localization of the atoms into the potential wells of the optical lattice. Finally, $I_0$, scaling the depth of the potential, represents the maximum number of photons an atom can scatter into the cavity

$$ I_0 = \frac{|\eta|^2}{|\Delta_c - N U_0 B|^2 + \kappa^2} . $$
It can be easily seen that a uniform distribution of atoms together with a zero coherent field inside the resonator is a trivial solution of the problem. Because \(<\cos kx> = 0\) for a constant atomic distribution, the cavity field driving term vanishes and \(\alpha_0 = 0\). There is no potential then, \(U_1 = U_2 = 0\), thus the uniform distribution remains a good solution. However, it may not be a stable solution for the atomic distribution, since density fluctuations can be amplified for adequately chosen parameters.

Self-organization is based on the effect of the \(\lambda\) periodic \(U_1\) potential term which involves a positive feedback mechanism. Let us set the detuning \(\Delta_C < -N|U_0|\) so that the sign of \(U_1\) becomes the opposite of the sign of \(\Theta\), cf. Eq. (3.2a). Consequently, if some \(\lambda\)-periodic density fluctuation yields \(\Theta > 0\) (i.e., more atoms happen to be near the even sites than near the odd ones), it produces a potential \(U_1 \cos kx\) (with \(U_1 < 0\)) which has minima at the even sites, thus attracting even more atoms there. Simultaneously, the \(\lambda\)-periodic optical lattice of atoms fulfills the Bragg-condition for constructive interference, \(<\eta(x)> \neq 0\), so the atoms can scatter pump photons into the cavity. The positive feedback requires then just that the parameters \(U_1\) and \(\Theta\) have opposite signs. This can be ensured by choosing the cavity detuning

\[
\Delta_C = NU_0 - \kappa,
\]

which is a sufficient but not necessary condition (because the bunching parameter is less than 1, the field could be tuned closer to resonance). The runaway solution is counteracted by the kinetic energy and the collisions (in a BEC), both trying to maximally spread the atomic distribution, hence there is a critical pump power above which the self-organization can occur.

The \(\lambda/2\) periodic \(U_2\) potential term does not discriminate between the even and odd sites. Above threshold, however, this term can have a significant role. If the condensate localizes around, say, \(kx = 0\), the \(\cos kx\) potential has maxima at \(kx = \pi\) and atoms are repelled from this region, which assists the self-ordering process. The \(\cos^2 kx\) potential term has always minima both at \(kx = 0\) and \(kx = \pi\), thus it counteracts the repulsion. For certain parameters it may occur that a secondary minimum appears and the adiabatic potentials form an asymmetric double well potential. So called ‘defect’ atoms scattering photons with ‘wrong’ phase can be trapped in the shallower traps. In the organized pattern, the emergence of secondary potential minima at the complementary sites depends on the ratio of the two potential terms in Eq. (3.1), namely on \(U_1/U_2\). For perfect localization \((\eta \rightarrow \infty)\), the condition for the possibility of stable defects is

\[
N|U_0| > \kappa,
\]
which is precisely the condition of strong collective coupling in cavity QED, where the collective line shift exceeds the cavity linewidth. For finite pumping strengths ($N\eta_t < \infty$), the ratio of the two potential terms is dependent on the order parameter $\Theta$, thus on the localization of the condensate wave function. Therefore, the above condition Eq. (3.7) should change with the pump strength $N\eta_t$, collision parameter $g_c$. Because $U_2/U_1 \propto \Theta \leq 1$, the larger the order parameter $\Theta$, the smaller $N|U_0|$ is needed for getting defects.

The above analysis of the mean-field potential predicts the occurrence of three phases in the system; i) a homogeneous phase, where the atomic cloud spreads uniformly along the cavity axis, and the corresponding mean photon number is zero, ii) a self-organized lattice, in which the atoms form a $\lambda$-periodic density grating, which Bragg scatters pump photons into the cavity, iii) self-organized lattice with defect atoms occupying lattice sites at a distance of $\lambda/2$ from the original lattice. In the following sections, I describe the realization of these phases in two other systems, as hinted in the beginning.

### 3.1 Self-organization of a thermal cloud in a ring cavity

In this Section, we generalize the previously discussed model for a one-dimensional ring resonator with two counterpropagating modes. It corresponds to the experimental setups used in [71, 83, 84]. As a generic difference to the correlated atomic recoil laser (CARL), we consider a transverse pump scheme, i.e. the particles are laser driven from a direction perpendicular to the resonator axis, instead of one-sided cavity pumping. This geometry has the virtue that the polarizing field is separated from the cavity modes mediating the multiple scattering between the particles.

#### 3.1.1 Model

We consider a gas of $N$ polarizable particles coupled to two degenerate optical modes of a ring resonator, described by the plane wave mode functions $f_1(x) = e^{ikx}$ and $f_2(x) = e^{-ikx}$, with coherent amplitudes $\alpha_1$ and $\alpha_2$. The scheme of the system is depicted in Fig. 3.1. The particles are driven by a pump laser oriented perpendicular to the cavity axis. For simplicity, we consider the system in one dimension: the atoms are supposed to be confined near the resonator axis by e.g. a strong dipole trap. The interaction is in the dispersive regime, i.e. the pump laser is very far detuned with respect to the resonance frequencies of the gas particles: no real excitations need take place. Thus, the model which describes the dynamics is a straightforward generalization of the dispersive model
Figure 3.1: Scheme of a ring resonator with two counterpropagating modes.

derived in Sec. 2.1.4. For two cavity modes, the electric field Eq. (2.13) is completed to \( E(x) = f_1(x)a_1 + f_2(x)a_2 + E_{\text{pump}} \), where the last pumping field term is assumed to be constant along the resonator axis ‘x’. The atoms redistribute photons by coherent scattering between the two modes and the pump field. This process feeds the cavity modes with an effective amplitude \( \eta \). One obtains the Hamilton operator of the system, by inserting the new electric field \( E(x) \) into the effective Hamiltonian (2.17) and summing up for atoms at positions \( x_j \) with momentum \( p_j \), where \( j = 1...N \). Assuming coherent field in the cavity modes with amplitudes \( \alpha_1 \) and \( \alpha_2 \), the corresponding equations of motion read

\[
\frac{d}{dt} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = A \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} - i \eta \sum_{j=1}^{N} \left( f_1^*(x_j) \right) + \sum_{j=1}^{N} \left( f_2^*(x_j) \right),
\]

using a formal vector notation, with the coupling matrix

\[
A = \begin{pmatrix} i(\Delta_C - NU_0) - \kappa & -iNU_0\sigma \\ -iNU_0\sigma^* & i(\Delta_C - NU_0) - \kappa \end{pmatrix}.
\]

The diagonal terms include the detuning between the pump laser and the cavity modes, \( \Delta_C = \omega - \omega_C \), the cavity decay rate \( \kappa \), and the shift of the cavity resonance with an amount of \( U_0 \) per atom. This shift is due to forward scattering and is related to the atomic properties by \( U_0 = -\omega_C\chi'/V \), where \( \chi' \) is the real part of the linear polarizability and \( V \) is the mode volume. The total frequency shift due to the gas, expressed in terms of a dimensionless collective coupling parameter \( \zeta = NU_0/\kappa \), will later be used to describe the density of the atom cloud (neglecting a filling factor). The off-diagonal terms, i.e. the
coupling between the cavity modes stems from the stimulated back reflection off the gas. This process is heavily dependent on the positions of the atoms, through the complex parameter \( \sigma = \frac{1}{N} \sum_j e^{-ikx_j} \) describing spatial order. Similar to the Debye-Waller factor, \( |\sigma| \) is 1 if the gas forms a perfect lattice with period of an integer multiple of \( \lambda/2 \), and less than 1 for a non-perfect lattice; for an equidistributed gas, it is \( |\sigma| \propto 1/\sqrt{N} \). The phase of \( \sigma \) gives \( x_0 \), the “position of the lattice” modulo \( \lambda/2 \), with the definition \( \sigma = |\sigma| e^{-2ikx_0} \).

Note that in contrast to the order parameter defined in Eq. (3.3) for a single mode cavity, here we shall use \( |\sigma| \) for characterizing the spatial order in the system, since \( \sigma \) is the primary quantity that appears in the equations.

Interaction between the gas and the cavity field lifts the degeneracy of the cavity modes. It is instructive to calculate the new eigenmodes of the cavity which are

\[
h_-(x) = \sin k(x - x_0) , \quad h_+(x) = \cos k(x - x_0) ,
\]

have nodes, and antinodes at \( x_0 + n\lambda/2 \), respectively. The corresponding amplitudes,

\[
\beta_- = ie^{ikx_0} \alpha_1 - ie^{-ikx_0} \alpha_2 , \quad \beta_+ = e^{ikx_0} \alpha_1 + e^{-ikx_0} \alpha_2 ,
\]

are not coupled by the interaction with the atom gas. The frequencies of the eigenmodes \( h_- \) and \( h_+ \) are shifted with respect to the empty cavity, giving the effective detunings

\[
\Delta_- = \Delta_C - (1 - |\sigma|)NU_0 , \quad \Delta_+ = \Delta_C - (1 + |\sigma|)NU_0 .
\]

With the atoms at fixed positions \( x_j \), the mode amplitudes take on the stationary values

\[
\beta_- = \frac{2\eta}{\Delta_- + ik} \sum_j \sin k(x_j - x_0) , \quad \beta_+ = \frac{2\eta}{\Delta_+ + ik} \sum_j \cos k(x_j - x_0) .
\]

If the atoms are uniformly distributed, both amplitudes vanish by destructive interference of the components scattered by different atoms (\( kx_0 \) is an arbitrary phase in this case). If the gas roughly forms a lattice with period \( \lambda \) (\( x_0 \) giving the position of the lattice modulo \( \lambda/2 \)), mode \( h_- \) will be weakly coupled, since it has nodes at the lattice points. On the contrary, mode \( h_+ \) has antinodes at the atomic positions and is driven by stimulated Bragg scattering off the gas [84, 77]. Therefore, from the viewpoint of self-organization the ring resonator can be simplified to an effective one-mode cavity that has a mode function \( \cos k(x - x_0) \). Nevertheless, the free position parameter \( x_0 \) reflects the continuous translation invariance of the ring cavity, which is not broken by the mirrors, but by the atomic distribution.

The possibility of optical trapping of high field seekers with negligible spontaneous emission loss requires large red detuning, whereby the resonance shift \( U_0 \) is negative. It is
known from cavity cooling theory that the pump field has to be detuned below the cavity frequency to ensure damped motional dynamics [63]. For large enough density ζ, however, if the gas forms a more and more periodic structure, |σ| increases from 0 to 1, and the frequency of mode \( h_+ \) may exceed the pump frequency, i.e. \( Δ_+ \) may become positive. This yields heating and instability of the gas. The effect is all the more prominent since at \( Δ_+ ≈ 0 \) the population of mode \( h_+ \) is resonantly enhanced. We will discuss ways to avoid this problem and the effect of the detuning \( Δ_C \) and the density \( ζ \) on the dynamics below.

Up to this point, the gas was considered as an inert background against which the dynamics of the cavity field takes place. Now we relax this assumption, and include the dynamics of the gas particles, which is slow on the timescale of equilibration of the cavity field, \( κ^{-1} \). This separation of the timescales allows us to treat the gas dynamics adiabatically, in a way reminiscent of the Born-Oppenheimer approximation for molecules: the motion of the gas particles is governed by the forces from the light field that depends on their positions.

In fact, we generalize the mean-field model presented in Section 2.2.1. For large number of atoms but each of them weakly coupled to the cavity modes, one can take the thermodynamic limit (where \( N, V → ∞ \), keeping the density \( N/V = \text{const} \)), and treat the atomic cloud by a mean field approach using a continuous position distribution \( p(x) \). Furthermore, by assuming that the gas has a finite equilibrium temperature \( T \), we can apply the canonical distribution, giving

\[
p(x) = \frac{1}{Z} \exp \left( -\frac{V(x)}{k_BT} \right), \tag{3.14}
\]

with the partition function \( Z \) ensuring normalization \( \int p(x)dx = 1 \). Microscopic calculations reveal that the temperature is on the order of \( k_BT = \hbar κ \), when cavity cooling is optimal. The mean-field potential \( V(x) \) is given by the last term of the effective Hamilton operator (2.17), when the steady-state coherent amplitudes \( α_1 \) and \( α_2 \) are substituted for the operators \( a_1 \) and \( a_2 \), respectively. In turn, using the eigenmodes \( h_-(x) \) and \( h_+(x) \) with the corresponding coherent fields \( β_- \) and \( β_+ \) we have

\[
V(x) = 2\hbar μ \left( \text{Re}β_-\sin k(x-x_0) + \text{Re}β_+\cos k(x-x_0) \right) + \\
\frac{1}{2} \hbar μ_0 \left( |β_+|^2 - |β_-|^2 \right) \cos 2k(x-x_0) + 2\text{Re}[β_+^*β_-] \sin 2k(x-x_0) \right). \tag{3.15}
\]

The first line corresponds to scattering from the pump into the cavity: if the gas forms a \( λ \)-periodic grating, this describes a potential with attractive points at the lattice sites,
i.e. the gas density maxima. The second line originates from multiple scattering between the running wave modes. This latter has a strong dependence on the density and causes deviations from a medium with linear refractive index: it attracts particles to maxima of the cavity field, and can create defects in the lattice, as explained later on.

Now since \( V(x) \) depends on the mode amplitudes \( \beta_- \) and \( \beta_+ \), and these latter depend on the distribution \( p(x) \) of the scatterers through Eqs. (3.13), Eq. (3.14) has to be solved self-consistently.

### 3.1.2 Results

As hinted in Sec. 2.2.1, we find the self-consistent solution for the implicit equation (3.14) by numerically iterating the atomic distribution \( p(x) \). For weak pump amplitude \( \eta_0 \), this solution is the uniform distribution of the gas, \( p(x) = \lambda^{-1} \). Above a certain threshold \( \eta_c \), the uniform distribution is no longer stable and a nontrivial \( p(x - x_0) \) builds up, with \( x_0 \) depending on the initial fluctuations.

Fig. 3.2(a) shows this transition with a plot of the spatial order \( |\sigma|^2 \) as a function of the pumping strength. The narrowing of the “self-organized” density distributions is shown in Fig. 3.2(b) using two specific values for the pump \( \eta_0 \) above threshold.

The critical pump amplitude \( \eta_c \) can be determined analytically by a stability analysis of the uniform distribution. Taking a periodic perturbation, \( p^{(0)}(x) = \lambda^{-1}(1 + \epsilon g(x)) \), with \( \epsilon \) infinitesimal and \( g(x + \lambda) = g(x) \), \( \int_0^\lambda g(x)dx = 0 \), we do one and only one iteration presented in the previous paragraph. The Fourier components of \( g(x) \) with period \( \lambda/2 \) determine \( x_0 \). The only relevant Fourier components of the perturbation are those with period \( \lambda \), as only these affect the amplitudes \( \beta_\pm \); we can therefore take \( p^{(0)}(x) = \lambda^{-1}[1 + \epsilon A \cos k(x - x_0) + \epsilon B \sin k(x - x_0)] \). The condition of stability then becomes that the magnitudes of \( A \) and \( B \) decrease during a single iteration of Eq. (3.14) to first order in \( \epsilon \). For both \( A \) and \( B \) this translates to the condition \( \eta_0 < \eta_c \), with the critical pump amplitude

\[
\eta_c = \sqrt{\frac{k_BT}{\hbar \kappa} \sqrt{\frac{\kappa |U_0|}{\zeta} \sqrt{\frac{\delta^2 + 1}{2|\delta|}}} \quad (3.16)}.
\]

Here we use \( \delta = (\Delta_C - NU_0)/\kappa \). The lowest pump power allowing for self-organization to happen is at the detuning \( \delta = -1 \), i.e. \( \Delta_C = NU_0 - \kappa \).

This light-matter system is of particular interest because of the highly nonlinear dependence of the dynamics on the density of atoms. At higher optical densities the self-consistent distribution \( p(x) \) which develops above the pump power threshold becomes
more complex. The order $|\sigma|^2$ as a function of the density parameter $\zeta$ at fixed pumping strength $\eta_t = 0.1\kappa$ is plotted in Fig. 3.3(a). In accordance with Eq. (3.16), below a critical density $\zeta_c$ the uniform distribution is stable.

At densities $\zeta > \zeta_c$, where the pump is above threshold, a rough but surprisingly good approximation is that the atoms form a perfect lattice, which from Eq. (3.15) gives for the potential:

$$ V(x) \approx -\hbar \frac{2Nk\eta_t^2}{\Delta_+^2 + \kappa^2} \left( -\frac{2\Delta_+}{\kappa} \cos k(x - x_0) + \zeta \cos 2k(x - x_0) \right). \quad (3.17) $$

This approximation holds when mode $h_-$ is hardly populated. The lattice is defined by the first term having attractive minima at $kx = kx_0 + 2n\pi$. Due to the second, density-dependent term, a secondary peak can build up at $kx = kx_0 + (2n+1)\pi$, roughly above $\zeta > -\Delta_C/(4\kappa)$. “Defect” atoms can then appear in the lattice which radiate into the cavity mode $h_+$ in opposite phase with the atoms being at $x_0$, thus decreasing the photon number. However, in a thermal distribution these sites are hardly occupied such that the order parameter does not indicate this transition, which is at $\zeta = 1$ in the numerical example of Fig. 3.3(a). The distribution $p(x)$ is still dominated by a single peak around $x_0$ whose width decreases with increasing pump power.

At even higher optical densities, pumping above the threshold results in an instability of the atom cloud – this is the reason why the curve in Fig. 3.3(a) is only plotted up to $\zeta = 2$. The iterations of Eq. (3.14) no longer converge, but enter a loop of flipping between two localized distributions which differ in a shift by $\lambda/2$. This indicates a frustration of the system: when more atoms happen to be, say, close to the positions $x = x_0 + n\lambda$, for
Figure 3.3: (a) Order parameter as a function of the density of cloud (expressed by the collective coupling $\zeta$) at a fixed pumping strength, $\eta_t = 0.1\kappa$, and detuning $\Delta_C = -4\kappa$. (b) The position distribution $p(x)$ showing “defect” atoms (solid line) and the self-consistent mean-field potential $V(x)$ (dashed line) for $\zeta = 2$, as indicated by the arrow on (a).

$\Delta_+ > 0$ they create a potential favoring the sites at $x = x_0 + (n + \frac{1}{2})\lambda$. The detuning $\Delta_+$ becomes positive at large pump power when $\zeta > -\Delta_C/(2\kappa)$, which in Fig. 3.3(a) corresponds to $\zeta > 2$. Note that in Fig. 3.3(b), presenting a still stable, but markedly two-peaked distribution, the potential depths at the two possible sites become very close to each other.

We summarize the numerical results on a phase diagram in Fig. 3.4. Choosing a fixed pump-cavity detuning, $\Delta_C = -4\kappa$, two parameters, namely the dimensionless optical density $\zeta$ and the pumping strength $\eta_t/\kappa$ determine the equilibrium distribution. A complete map of sharply separated regimes, “uniform distribution”, “self-organized lattice”, “lattice with defects” and “no convergence”, are presented. The overall $\eta_c \propto \zeta^{-1/2}$ dependence of the stability limit of the uniform distribution, according to Eq. (3.16), shows up clearly in this log-log plot. The unstable region is cut by a sharp resonance at $\zeta = 4$, which corresponds to the density where the detuning $\Delta_C = NU_0$. In accordance with Eq. (3.16), this density leads to $\delta = 0$ and yields a divergence of the critical pump amplitude. For this setting the uniform distribution is stable against infinitesimal perturbations, no matter how strong the laser pump is. Finite fluctuations can, however, be amplified and for strong pumping the uniform distribution does become unstable. The other region boundaries are in good agreement with the analytical results for large $\eta_t$ ($\zeta \approx 1$ and $\zeta \approx 2$).
3.1.3 Summary

By mean-field analysis I revealed the various phases of an ensemble of cold atoms which are strongly coupled to the radiation modes of a lossy ring cavity and off-resonantly driven by a transverse laser. The interaction of linearly polarized particles with light is demonstrated to be strongly nonlinear in the large intensity and large density limit. A complete phase diagram has been obtained as a function of the transverse pump amplitude and the collective coupling strength, where the phase boundaries are interpreted by simple physical arguments. In the next section, I shall reveal similar phases for a Bose-Einstein condensate inside a single-mode optical resonator that provides an opportunity to compare self-organization in the two systems.
3.2 Self-organization of a Bose-Einstein condensate in an optical cavity

In this section, we study the self-organization phenomenon in the case of coupled matter and radiation fields. As a first step in understanding the complex dynamics of this system, we neglect quantum statistical effects [109, 110] and resort to a mean field approximation. We adopt the model developed by P. Horak et al. [108] for a different geometry. In their scheme, the coherent laser field was injected directly into the cavity. Then the transition between homogeneous and periodically modulated densities is smooth as a function of the external pump power. By contrast, we consider the case of illuminating directly the atoms, which yields a phase transition, i.e., an abrupt change of the stationary state of the system at a well-defined threshold pump power. Note the delicate difference between stationary state and ground state of the system. The condensate does not follow a coherent Hamiltonian dynamics because of the coupling to the decaying cavity field. The total system is dissipative owing to the irreversible photon loss from the cavity. Thus we have to consider the steady-state of a driven open system far from equilibrium and perturbations around this steady-state.

3.2.1 Model

We describe the coupled BEC–cavity system in terms of the mean-field model derived in Section 2.2.2. For completeness, however, we briefly summarize the model assumptions and describe the origin of the effective parameters of the system.

We consider a pure Bose-Einstein condensate (BEC) interacting with a single-mode of a high-\(Q\) optical cavity. The condensate atoms are coherently driven from the side by a laser field with frequency \(\omega\), directed perpendicularly to the cavity axis. The laser is detuned far from the atomic transition \(\omega_A\), that is, \(|\Delta_A| \gg \gamma\), where \(2\gamma\) is the full atomic linewidth at half maximum and the atom-pump detuning is \(\Delta_A = \omega - \omega_A\). This condition ensures that the electronic excitation is extremely low in the condensate atoms, hence the spontaneous photon emission is suppressed. At the same time, the laser field is nearly resonant with the cavity mode frequency \(\omega_C\), i.e. \(|\Delta_C| \approx \kappa\), where \(\kappa\) is the cavity mode linewidth and the cavity-pump detuning is \(\Delta_C = \omega - \omega_C\). The scattering of laser photons into the cavity is thus a quasi-resonant process and is significantly enhanced by the strong dipole coupling between the atoms and the mode due to the small volume of the cavity. This coupling strength is characterized by the single-photon Rabi frequency.
$g_0$, which is in the range of $\kappa$. Therefore, although the condensate is hardly excited, it can efficiently scatter photons into the cavity.

For the sake of simplicity, we describe the dynamics in one dimension $x$ along the cavity axis. The cavity mode function is then simply $\cos kx$. This model can apply e.g. to a cigar shaped BEC tightly confined in the transverse directions by a strong dipole or magnetic trap, so that the transverse size of the condensate $w$ is smaller than the waist of the cavity field. The pump laser is assumed to be homogeneous along the cavity axis therefore it is described by a constant Rabi frequency $\Omega$.

The condensate contains a number of $N$ atoms assumed to have the same wave function $|\psi(t)\rangle$. The cavity field is assumed to be in a coherent state described by the complex amplitude $\alpha$. These approximations imply that the quantum state of the system is factorized: entanglement between the condensate and the cavity field [111, 112] is neglected, which can be done for large enough cavity photon number $|\alpha|^2$.

The cavity field is subject to the strong refractive index effect of the optically dense condensate. At the same time, the evolution of the condensate wave function is described by a Gross-Pitaevskii-type equation, including the mechanical effect of the radiation field in the cavity. The system of coupled mean-field equations is readily derived in Eqs. (2.26), which read

\begin{equation}
    i \frac{\partial}{\partial t} \alpha = [-\Delta_c + N\langle U(x) \rangle - i\kappa] \alpha + N\eta(x),
\end{equation}

\begin{equation}
    i \frac{\partial}{\partial t} \psi(x,t) = \left\{ \frac{\hbar^2}{2m} U(x) + |\alpha(t)|^2U(x) + 2\Re\{\alpha(t)\}\eta(x) + Ng_c|\psi(x,t)|^2 \right\} \psi(x,t).
\end{equation}

Let us discuss the physical meaning of the terms coupling the photon and the matter fields. Each atom shifts the cavity resonance frequency in a spatially dependent manner by $U(x) = U_0 \cos^2 kx$. The maximum shift is $U_0 = g^2/\Delta_A$, obtained at the antinodes of the mode function. In the mean-field approximation, the shift has to be spatially averaged over the single-atom wave function, giving the frequency shift per atom $\langle U(x) \rangle = U_0 \langle \psi | \cos^2 kx | \psi \rangle$. It is worth noting that, even if the one-atom light shift $U_0$ is small compared to the cavity decay $\kappa$, one can achieve the interesting strong collective coupling regime of cavity QED, $N|U_0| > \kappa$, with a trapped BEC. Feeding the cavity by laser scattering on the atoms appears as an effective pump with strength $\eta_t = \Omega g^2/\Delta_A$. This process has a spatial dependence inherited from the mode function, $\eta_t(x) = \eta_t \cos kx$, and this term also has to be averaged over the condensate wave function.

The well known Gross-Pitaevskii equation (GPE) in one dimension in Eq. (3.18b) describes the motion of a scalar condensate induced by the optical forces in the cavity
field. The back action of the light shift is the term proportional to $U(x) = U_0 \cos^2 kx$ and the cavity photon number $|\alpha|^2$. This term is periodic with half of the wavelength $\lambda$ and, in free space, is referred to as an “optical lattice”. The back action of the coherent scattering of photons between the transverse pump and the cavity mode is the term proportional to $\eta_l(x) = \eta_l \cos kx$ and has a periodicity of $\lambda$. The last term of the GPE accounts for the s-wave collision of the atoms, its strength is related to the s-wave scattering length $a$ by

$$g_c = 4\pi\hbar a/(mw^2),$$

and depends on the transverse size $w$ of the condensate. We assume repulsive atom–atom collisions in the system ($a > 0$) which are necessary to maintain the stability of the condensate in the thermodynamic limit [106]. In the following we will consider the case $U_0 < 0$, i.e. large red detuning, where the atoms behave as high field seekers. Consequently, for nonzero cavity field the condensate atoms tend to localize around the field antinodes, thereby maximizing their coupling to the light field.

It can be checked that Eqs. (3.18) with the field amplitude replaced by $\alpha/\sqrt{N}$ are invariant under the scaling of the parameters such that $NU_0$, $N\eta_l$, and $\sqrt{N}\eta_l$ is kept constant. That is, in the mean field model, the atom number can be incorporated in the system parameters and the field amplitude variable (with the proposed rescaling, the absolute square of this latter gives the photon number per atom). Therefore, in the following the system parameters will occur only in the form of the above combinations. However, we refrain from introducing a new notation for the scaled parameters in order to signify their relation to experimental parameters.

Further simplification for the numerical method can be obtained by making use of the periodicity of the optical potential. We can consider periodic wave functions $\psi(x)$, and solve Eqs. (3.19) in the interval $[0, \lambda]$ using periodic boundary condition. In this way, we discard the dynamics within a “Bloch band”. We are interested in effects due to the condensate-cavity field interaction which does not couple states of different quasi momenta. Hence it is independent of the length of the interval and we choose the shortest one to reduce the computational effort. By contrast, the collisional interaction depends on the actual atom density, hence, for a fixed atom number $N$, the density is artificially enhanced by folding the space into a single $\lambda$ interval. Therefore, the collision parameter has to be modified such that $N\gamma_c/\lambda$ correspond to the collisions at the actual (experimental) atom density in the cavity.
3.2.2 Steady state

In the first place, we intend to study the steady state of the compound condensate-cavity system. It is described by the field amplitude $\alpha_0$, and the condensate wave function $\psi(x, t) = \psi_0(x)e^{-i\mu t}$, where $\hbar \mu$ is the chemical potential. Following from Eq. (3.18), they obey the system of equations

$$\alpha_0 = \frac{N \langle \psi_0 | \eta_t(x) | \psi_0 \rangle}{\Delta_C - N \langle \psi_0 | U(x) | \psi_0 \rangle + i\kappa}, \quad (3.19a)$$

$$\left\{ \frac{p^2}{2\hbar} + |\alpha_0|^2 U(x) + 2\text{Re}\{\alpha_0\eta_t(x) + N g_c |\psi_0(x)|^2 \} \right\} \psi_0(x) = \mu \psi_0(x). \quad (3.19b)$$

The solution for $\psi_0(x)$, $\mu$ and $\alpha_0$ can be determined in a self-consistent manner. As discussed in Section 2.2.2, we calculate the steady state numerically by using a variant of the imaginary time propagation method.

Since the mean-field model of the condensate is closely related to the mean-field model of a thermal gas of atoms presented in Sec. 2.2.1, one can expect that the phase transition appears as an abrupt change of the self-consistent steady state at a critical pumping strength $\eta_t$. The physical process is analogous, however, at zero temperature the kinetic energy and the atom-atom collisions are apt to stabilize the phase with larger symmetry.

The relevant parameters are measured in units of the recoil frequency $\omega_R = \hbar k^2/(2m)$ and in units of the recoil energy $\hbar \omega_R$. The natural length scale is the optical wavelength $\lambda$ of the cavity field. We set the strength of the s-wave interaction $N g_c = 10 \omega_R \lambda$. The atom-cavity coupling is characterized by $N U_0 = 100 \omega_R$, which is on the order of the cavity decay rate, $\kappa = 200 \omega_R$. We set the value of the cavity detuning, according to Eq. (3.6), $\Delta_C = -300 \omega_R$.

The numerical solution for the self-consistent ground state of the condensate-cavity system confirms the qualitative agreement with the thermal gas. In Fig. 3.5, the appearance of the self-organized lattice is manifested by the variation of the order parameter $\Theta = \langle \psi_0 | \cos kx | \psi_0 \rangle$ against the pumping strength $\sqrt{N} \eta_t$ (compare, e.g. with Fig. 3.2).

Above a critical pump amplitude ($\sqrt{N} \eta_t \approx 65.6 \omega_R$), the homogeneous condensate, our initial guess for the condensate wave function, self-organizes into a lattice of period $\lambda$. At the outset of the self-organization, a spontaneous symmetry breaking occurs: the condensate occupies either the $kx = 0$ site or the $x = \pi$ site. Further increasing the pump strength $\sqrt{N} \eta_t$, the atoms get more and more localized around the chosen site, that is indicated by the growth of the order parameter $\Theta$. The localization of the condensate
Figure 3.5: Left: The order parameter \( \Theta \), plotted as a function of the transverse pump amplitude \( \sqrt{N}\eta_h \), exhibits the self-organization of the BEC into a \( \lambda \)-periodic optical lattice. Right: Two typical atomic position distributions \( |\psi_0(x)|^2 \) (solid lines) and the corresponding adiabatic optical potentials from Eq. (3.1) (dashed lines) for pump strengths \( \sqrt{N}\eta_h = 100\omega_R \) (thick lines) and \( \sqrt{N}\eta_h = 300\omega_R \) (thin lines). The other parameters are \( Ng_c = 10h\omega_R\lambda \), \( NU_0 = -100\omega_R \), \( \Delta_C = -300\omega_R \), \( \kappa = 200\omega_R \).

In the self-organized phase is showed on the right of Fig. 3.5 for two specific transverse pump amplitudes \( \sqrt{N}\eta_h = 100 \) (thick lines) and \( 300\omega_R \) (thin lines).

The critical pump amplitude \( \sqrt{N}\eta_c \) can be determined analytically by the stability analysis of the trivial solution of Eqs. (3.19), being \( \psi_0(x) \equiv 1 \), \( \alpha_0 = 0 \), \( \mu_0 = Ng_c \). Only the Fourier component \( \cos kx \) of a noisy perturbation of the wave function can produce a non-vanishing cavity field \( \alpha_0 \) other than zero, in accordance with the mean value \( \langle \psi | \cos kx | \psi \rangle \) in the numerator of Eq. (3.19a). Therefore, starting from the wave function \( \psi(x) = 1 + \epsilon \cos kx \), with \( \epsilon \ll 1 \), we carry out one iteration step of the imaginary time propagation method:

\[
\frac{\Delta \psi}{\Delta \tau} = -Ng_c - \epsilon \cos kx \times \left( \omega_R + N\eta_h^2 \frac{2\Delta_C - NU_0}{(\Delta_C - NU_0/2)^2 + \kappa^2} + 3Ng_c \right). 
\]

(3.20)

The component \( \psi_0 = 1 \) decays with the rate \( \mu_0 = Ng_c \), while the decay of the perturbation \( \cos kx \) depends on the pumping strength \( \eta \). In order to preserve the stability of the homogeneous ground state, the perturbation should decay faster than \( \psi_0 \). The condition that the coefficient of \( \epsilon \cos kx \) is equal to \( Ng_c \) leads to the critical pump amplitude

\[
\sqrt{N}\eta_c = \sqrt{\frac{(\Delta_C - NU_0/2)^2 + \kappa^2}{(NU_0 - 2\Delta_C)^2}} \sqrt{\omega_R + 2Ng_c}.
\]

(3.21)

Interestingly, the critical pump amplitude given by Eq. (3.21) is formally analogous to the one obtained in the case of a thermal classical gas in Section 3.1. However, the
temperature is substituted by the kinetic energy and the s-wave collision of the atoms, formally \( k_B T/\hbar \leftrightarrow \omega_R + 2Ng_c \).

### 3.2.3 Collective excitations

Let us now calculate the excitation spectrum of the coupled condensate-cavity system as the linear response of the self-consistent steady-state. Two limiting cases can be relatively easily understood: (i) for \( \eta_t = 0 \) there is no field in the cavity and one gets back the excitation spectrum of a homogeneous Bose-gas; (ii) for \( \eta_t \rightarrow \infty \), deeply in the self-organized phase, where the optical potential can be approximated as a parabola, one expects to obtain the excitations of a BEC in harmonic trap potential. This simplification, however, does not perfectly apply since the excitations are not only collective oscillations of the atom cloud, but they are polaritons involving the fluctuation of the field amplitude around its steady state. In the following, we will consider the full transition range, including the critical point, between these limiting cases.

We need to consider the deviations from the stationary state (\( \psi_0 \) and \( \alpha_0 \)):

\[
\alpha(t) = \alpha_0 + \delta \alpha(t) ,
\]

\[
\psi(x, t) = e^{-i\mu t}[\psi_0(x) + \delta \psi(x, t)] .
\]

Inserting the ansatz into Eqs. (3.18) and linearizing in \( \delta \psi \) and \( \delta \alpha \), one gets

\[
i\delta \dot{\alpha} = A\delta \alpha + N\alpha_0[\langle \psi_0 | U(x) | \delta \psi \rangle + (\delta \psi | U(x) | \psi_0) - N[\langle \psi_0 | \eta_t(x) | \delta \psi \rangle + (\delta \psi | \eta_t(x) | \psi_0) ,
\]

\[
i\delta \dot{\psi} = \{H_0 + Ng_c|\psi_0(x)|^2 \} \delta \psi + Ng_c\psi_0^2(x)\delta \psi^*
\quad + \psi_0(x)U(x)(\alpha_0\delta \alpha^* + \alpha_0^*\delta \alpha) + \psi_0(x)\eta_t(x)(\delta \alpha + \delta \alpha^*) ,
\]

where

\[
A = -\Delta C + N \langle \psi_0 | U(x) | \psi_0 \rangle - i\kappa ,
\]

and

\[
H_0 = \frac{p^2}{2\hbar m} + Ng_c|\psi_0(x)|^2 - \mu + |\alpha_0|^2U(x) + 2Re\{\alpha_0 \}\eta_t(x) .
\]

Because the linearized time evolution couples \( \delta \psi \) and \( \delta \alpha \) to their complex conjugates, we search the solution in the form

\[
\delta \alpha(t) = e^{-i\omega t} \delta \alpha_+ + e^{i\omega^* t} \delta \alpha_- ,
\]
\[ \delta \psi(x, t) = e^{-i\omega t} \delta \psi_+(x) + e^{i\omega t} \delta \psi_-(x), \]  

(3.25b)

where \( \omega = \nu - i\gamma \) is a complex parameter of the oscillation standing for frequency \( \nu \) and damping rate \( \gamma \). Equations (3.23) have to be obeyed separately for the \( e^{-i\omega t} \) and \( e^{i\omega t} \) terms, which leads to the linear eigenvalue equation:

\[
\begin{bmatrix}
\delta \alpha_+ \\
\delta \alpha_- \\
\delta \psi_+(x) \\
\delta \psi_-(x)
\end{bmatrix} = M \begin{bmatrix}
\delta \alpha_+ \\
\delta \alpha_- \\
\delta \psi_+(x) \\
\delta \psi_-(x)
\end{bmatrix},
\]

(3.26)

where \( M \) is a non-Hermitian matrix being determined by Eqs. (3.23). Collective excitations of the system are the solutions of this eigenvalue problem. It simplifies if we choose \( \psi_0(x) \) real, and write \( M \) in the basis of the symmetric and antisymmetric combinations,

\[
\begin{align*}
\delta \alpha_a &= \delta \alpha_+ - \delta \alpha_- , \\
\delta \alpha_s &= \delta \alpha_+ + \delta \alpha_- , \\
\delta f(x) &= \delta \psi_+(x) + \delta \psi_-(x) , \\
\delta g(x) &= \delta \psi_+(x) - \delta \psi_-(x).
\end{align*}
\]

(3.27)

Transformed into this basis, the matrix \( M \) is

\[
\begin{bmatrix}
-i\kappa & \text{Re}A & 2N(\text{Re}a_0X + Y) & 0 \\
\text{Re}A & -i\kappa & 2iN\text{Im}a_0X & 0 \\
0 & 0 & 0 & -H_0 \\
2i\psi_0U\text{Im}a_0 & -2\psi_0(U\text{Re}a_0 + \eta_t) & -H_0 - 2Ng_c\psi_0^2 & 0
\end{bmatrix} .
\]

(3.28)

The argument \( x \) has been omitted from the functions \( \psi_0, U \) and \( \eta_t \) for brevity. The integral operators \( X \) and \( Y \), coupling the condensate excitations to the cavity field, read

\[
X \xi(x) = \int dx \psi_0(x)U(x)\xi(x), \quad (3.29a)
\]

\[
Y \xi(x) = \int dx \psi_0(x)\eta_t(x)\xi(x). \quad (3.29b)
\]

Being a non-Hermitian matrix, \( M \) has different right and left eigenvectors corresponding to the same eigenvalue \( \omega \).

The matrix has a special symmetry: if \( \omega \) is an eigenvalue with the right eigenvector

\[
(\delta \alpha_a, \delta \alpha_s, \delta f, \delta g),
\]
then $-\omega^*$ is also an eigenvalue with the right eigenvector
\[ (-\delta \alpha_n^*, \delta \alpha_n^*, \delta f^*, -\delta g^*). \]

Thus the eigenvalues come in pairs, having the same imaginary parts but the real parts are of the opposite sign in a pair. This grouping of the eigenvectors makes sense for eigenvalues with non-vanishing real part.

The imaginary part describes damping which arises from the nonadiabaticity of the cavity field dynamics. The linear perturbation calculus of the excitations which we adopted here takes into account that the field follows the changes of the BEC wave function with a delay in the order of $1/\kappa$. Depending on the specific choice of the parameters, this can yield damping or heating, which is known as cavity cooling and has been extensively studied in the past decade. Damping of BEC excitations in optical cavities, which has been first studied in Refs. [108, 113], is an interesting opportunity which motivates the realization and the study of the coupled cavity-condensate system.

Spectrum analytically below threshold

Below threshold, the condensate wave function is constant and linearization around this simple solution leads to analytical results. The stability of the uniform distribution can be evaluated from the spectrum, thus the critical point can be determined in this way, independently of the previous calculation in Sec. 3.2.2. Moreover, we obtain a detailed description of a restricted part of the spectrum which contains polariton excitations.

Assuming homogeneous atomic distribution and, correspondingly, vanishing cavity field ($\psi_0 \equiv 1, \alpha_0 = 0$), the only non-trivial coupling term in the matrix $M$, see Eq. (3.28), is the $Y$ operator defined in Eq. (3.29b). Since $\eta_l(x) \propto \cos kx$, only the Fourier component $\cos kx$ couples to the cavity amplitude. In return, the fourth line of the matrix $M$ shows that the field fluctuations excite just this $\eta_l(x) \propto \cos kx$ condensate perturbation. Thus, this subspace is closed below threshold. All the other condensate excitations decouple from the field and remain simply the higher Fourier components with frequencies
\[ \Omega_n = \sqrt{n^2 \omega_R (n^2 \omega_R + 2Ng_c)}, \quad (n > 1), \quad (3.30) \]

which is identical to the excitations of a homogeneous condensate in a box [106]. It is
sufficient to diagonalize the matrix $M$ in the restricted subspace,

$$
\begin{pmatrix}
-\i & \delta_C & N\eta_t & 0 \\
\delta_C & -\i & 0 & 0 \\
0 & 0 & -\omega_R & 0 \\
0 & -2\eta_t & -\omega_R - 2Ng_c & 0
\end{pmatrix}.
$$

(3.31)

It has the fourth order characteristic equation

$$
(\lambda^2 - \Omega_1^2) \left[ (i\kappa + \lambda)^2 - \delta_C^2 \right] - 2N\eta_t^2\omega_R\delta_C = 0,
$$

(3.32)

where $\delta_C = -\Delta_C + \frac{1}{2}NU_0$, and $\Omega_1$ is the first excitation energy in the Bogoliubov spectrum (3.30) of a BEC in a box. One can check that, for $\eta_t = 0$, the last term vanishes and $\lambda_{1,2} = \pm\Omega_1$ for the condensate excitation, $\lambda_{3,4} = \pm\delta_C - i\kappa$ for the cavity mode. For non-zero pumping, $\eta_t \neq 0$, the condensate-like and the field-like excitations mix. When $\Omega_1^2 \ll \kappa^2 + \delta_C^2$, the frequencies corresponding to the excitations of the free field and to the free condensate are well separated. Therefore, the mixing ratio is small so that the polariton modes can be attributed to dominantly condensate or field excitations.

At the onset of self-organization the uniform ground state $\psi_0$ changes, which, in the present approach, corresponds to the appearance of a zero eigenvalue in the spectrum. In Fig. 3.6, we plot the numerical solutions of Eq. (3.32) for the lowest, dominantly condensate-type excitation. The real parts (solid red) tend to zero as increasing the pump strength. Oppositely, the absolute value of the imaginary parts of the eigenvalues (dashed green) increases with the pump strength. The behaviour of the eigenvalues near the critical point $\sqrt{N}\eta_c = 65.612\omega_R$ is magnified in the inset of Fig. 3.6. When the real parts reach zero at $\sqrt{N}\eta_c$, the initially identical imaginary parts split up and the upper branch crosses zero. This crossing is the critical point, here the $\psi_0$ steady-state becomes dynamically unstable. By expressing $\eta_t$ from Eq. (3.32) for $\lambda = 0$, the same critical transverse pump amplitude $\eta_c$ is obtained as that in Eq. (3.21).

The emergence of a positive and a negative imaginary part just at the vanishing of the real parts of an excitation is a typical feature of a condensate’s instability. In our case, however, coupling to the cavity field yields a negative imaginary part where the real part becomes zero. Thus, there is a narrow range, as shown by the inset of Fig. 3.6, where the real parts remain zero, but both imaginary parts are negative. This unfamiliar course of the dynamical instability is a signature of cavity cooling, thus it is so for finite cavity decay rate $\kappa$. 

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Figure 3.6: Eigenvalues of the lowest condensate excitation of a homogeneous BEC from Eq. (3.32) as a function of the pump strength $\sqrt{N\eta_t}$. As shown in the inset, the real parts (solid red) vanishes slightly below the critical point which is reached when the upper branch of the imaginary parts (dashed green) crosses zero. In the main figure the imaginary parts are magnified by a factor of 50. Parameters are the same as in Fig. 3.5.

In the limit $\Omega_1^2 \ll \kappa^2 + \delta_C^2$, the first excitation frequency can be approximated by

$$\text{Re}\lambda_1 = \Omega_1 \sqrt{1 - \frac{\eta_c^2}{\eta_c^0}}, \quad \text{(3.33a)}$$

and the imaginary part is quadratic in the pump strength,

$$\text{Im}\lambda_1 = -\frac{\kappa \Omega_1^2}{\delta_C^2 + \kappa^2} \frac{\eta_c^2}{\eta_c^0}. \quad \text{(3.33b)}$$

These approximate expressions fit well the curve shown in Fig. 3.6. The s-wave interaction between atoms increases the decay rate of this particular excitation. The imaginary part vanishes, of course, for $\kappa \to 0$.

The width of the narrow range, where the $\psi_0 = 1$ uniform steady state is stabilized by that the cavity cooling damps out zero-energy excitations, is obtained:

$$\eta_c^2 - \eta_c^0 = \eta_c^0 \left( \frac{\kappa \Omega_1}{\delta_C^2 + \kappa^2} \right)^2. \quad \text{(3.34)}$$

Similarly to the decay rate $\text{Im}\lambda_1$, the range expands on increasing the collisional parameter $N g_c$. Finally, note that Eq. (3.34) is considered a small parameter in the estimation of $\lambda_1$ in Eqs. (3.33).
Figure 3.7: Frequencies (a) and decay rates (b) of the six lowest collective condensate excitations and the ones corresponding to the cavity field as a function of the transverse pump strength. Decay rates of the lower branches of each pair are 0. For the cavity-dominated mode the frequency and the decay rate is divided by 5 and 4000, respectively, and $\gamma_1$ is divided by 2 in (b). Parameters are the same as in Fig. 3.5.

**Full spectrum**

Above threshold, the collective condensate-cavity excitations belong to the self-consistent ground state given by Eqs. (3.19) which can be calculated only numerically. Therefore, the solution of the eigenvalue problem in Eq. (3.26) is performed also numerically using LAPACK. The wave function is defined on a spatial grid of 200 points in the interval of one wavelength.

In Fig. 3.7(a), we show the first three excitation frequencies and damping rates ($\gamma_1/2$ is plotted) of the condensate around the real ground state, and the frequency and damping rate of a higher excited state corresponding to the cavity mode (double dashed lines, $\nu_f/5$ and $\gamma_f/4000$ are plotted). We depict only the positive frequencies, taking into account the symmetry of the eigenvalues of the matrix (3.28).

Below threshold the wave function $\psi_0(x)$ is constant, only the first excitation $\cos kx$ couples to the cavity field, and tends to zero on increasing the pumping, as it has been discussed before. All the other excitations are independent of the field, and have constant energies giving back the Bogoliubov excitation spectrum of a condensate in a box, see Eq. (3.30). Two orthogonal excitations have a fixed number of nodes and are degenerate in this regime. One of the modes in each pair is orthogonal to the cavity mode function $\cos kx$, thus decouples from the cavity field.

At the onset of self-organization the eigenvalues dramatically change. At the criti-
cal point the excitation energies drop slightly below the Bogoliubov energies given in Eq. (3.30). This dip is related to the collisions and disappears for \( g_c \rightarrow 0 \). Let us mention that the numerical calculation of the stationary solution of the Gross-Pitaeskii equation becomes inaccurate at the critical point. The convergence of the iterative solution slows down, which is an inherent consequence of the criticality obtained at the degeneracy of the ground and first excited state energies. Nevertheless we checked in some points that the dip is still there if very high accuracy is demanded in the iteration process.

At threshold, the degeneracy in the excitation pairs is lifted. The lower branch remains orthogonal to the cavity mode and decouples from the field fluctuations. The upper branches correspond to polariton excitations mixing condensate and field fluctuations.

Far above threshold, \( \sqrt{N} \eta \rightarrow \infty \), the excitation frequencies increase linearly with \( \sqrt{N} \eta \) and are uniformly spaced. This can be understood if we approximate the deep optical trap by a harmonic potential in the vicinity of the antinodes. The adiabatic potential in Eq. (3.1), transformed by using \( \cos kx \approx 1 - (kx)^2/2 \), gets a characteristic harmonic frequency proportional to the square root of the intracavity intensity. Thus, from Eq. (3.5), the trap frequency is linearly proportional to \( \sqrt{N} \eta \). The spectrum is composed of the integer multiples of this frequency. This is obvious in the collisionless case, \( g_c = 0 \), where the excitation frequencies are the same as for a single particle in a harmonic potential. The other extreme case, the Thomas-Fermi regime which we are closer to with the parameters of Fig. 3.7, can also be treated. Here, for a three-dimensional harmonic trap the excitation frequencies are given by a linear combination with integer coefficients of the three vibrational frequencies [114]. This can be contracted to one dimensional motion by assuming very large frequencies in the transverse directions, then the low excitations are obtained as integer multiples of the longitudinal trap frequency.

In Fig. 3.7(b), the decay rate of the excitations corresponding to the upper branches in Fig. 3.7(a) are shown. The lower branch of each pair has zero damping because it is orthogonal to the mode function of the cavity field. The lowest excitation decays with a rate \( \gamma_1 \) which exhibits a dip at threshold. In principle, it should drop down to zero, as shown in Fig. 3.6 representing the exact result below the critical point, however, the accuracy of the numerical calculation breaks down in the vicinity of the threshold due to critical slowing down. Somewhat above threshold, \( \gamma_1 \) rises back to the value it had below threshold and then increases further with increasing \( \sqrt{N} \eta \). Not too far above threshold, the weakly localized ground state enables the coupling of higher condensate excitations to the cavity field. These modes become damped, but their damping rate vanishes in the \( \sqrt{N} \eta \rightarrow \infty \) limit. There, as the ground state tends to a tightly localized one in a
harmonic trap, only the second excitation is coupled to the field [108].

The frequency and the decay rate of the cavity field are weakly perturbed by the condensate. The frequency of the cavity mode is expected to be \( \nu_f = \Delta_C - NU_0B \), that depends on the collective coupling \( NU_0 \) and, through the bunching parameter, on the localization of the ground state \( \psi_0 \). Decrease in the field mode frequency is accompanied by an increase of the stationary photon number \( |\alpha_0|^2 \) in the cavity.

### 3.2.4 Strong collective coupling regime

The interpretation of self-organization in terms of the adiabatic optical potential Eq. 3.1 in the introduction of this chapter reveals that the effect relies on the discrimination between the sites \( kx = 0 \) and \( kx = \pi \) (even and odd sites). The symmetry breaking is attributed entirely to the \( \lambda \) periodic potential. The other, \( \lambda/2 \) periodic \( \cos^2 kx \) potential, however, has always minima both at the even and the odd sites. As a result, secondary minima can appear in the total potential which counteract the Bragg scattering off the self-organized \( \lambda \)-periodic lattice. It is shown in Ref. [78] that for perfect localization \( (\eta_t \to \infty) \), defects can appear when

\[
N|U_0| > \kappa .
\]  

This condition corresponds to the strong collective coupling regime, where the collective light shift of the gas \( NU_0 \) exceeds the linewidth of the cavity resonance \( \kappa \). When the localization is not perfect, i.e., the order parameter \( \Theta \) is less than 1, larger \( N|U_0| \) is needed for getting defects.

The numerically exact critical lines are plotted in Fig. 3.8 below which the secondary potential minima appear as a function of the pumping strength for two different values of the s-wave collision parameter \( g_c = 0 \) and \( Ng_c = 10\lambda\omega_R \). The cavity detuning is fixed to \( \Delta_C = -2\kappa \). When collisions are not negligible, one needs a larger light shift \( N|U_0| \) to reach the regime where defects are expected, just because the collisions reduce the order parameter \( \Theta \). The vertical asymptote of the curves is at the threshold of the self-organization, while the horizontal one is at the same value defined by Eq. (3.35) that describes the \( \sqrt{N}\eta_t \to \infty \) behaviour for perfect localization.

Now let us turn to the effect of the secondary potential minima on the collective excitation spectrum. In the regime where the energy difference between the two types of potential minima is in the order of their depths, the lowest excitation energies in the deeper wells are comparable to those in the secondary ones. There will be collective
excitations that are composed of the combination of excitations localized in the two different wells.

For simplicity, we calculate the spectrum in the collisionless case for $g_c = 0$. In Fig. 3.9, we plot the collective excitation frequencies (a) and the decay rates (b) as a function of the pumping strength $\eta_t$ for $\kappa = 200\omega_R$ and $NU_0 = -1000\omega_R$. Starting from the Bogoliubov spectrum of the homogeneous condensate, there appear two types of excitation modes in the self-organized phase. The excitations that are localized in the deeper wells are the same as the ones presented in Fig. 3.7. Notice the lack of the dip at the critical point, which is because of the choice $g_c = 0$. The other type, represented by the two excitation modes bending up in Fig. 3.9a contain the excitations of the ‘defect’ well. For perfect localization, both the lower and the higher potential minima, hence also their difference, are proportional to $N|\eta_t|^2$. Exciting the condensate into the defect well costs the energy difference, this is the reason of the quadratic behavior as a function of the pumping strength $\sqrt{N}\eta_t$.

In order to exemplify the effect of the secondary potential minima in the spectrum,
Figure 3.9: Frequencies (a) and decay rates (b) of the six lowest collective condensate excitations in the regime, where the secondary potential minima are present as a function of the transverse pump strength. Decay rate of the first excitation $\gamma_1$ (solid red) is divided by 40. Parameters are $g_c = 0$, $NU_0 = -1000 \omega_R$, $\kappa = 200 \omega_R$ and $\Delta_C = -1200 \omega_R$.

we plot the wavefunctions of two condensate excitations at increasing values of the pump strength $\sqrt{N} \eta_l$ in Fig. 3.10. Namely, we chose the excitations with the lowest and the highest frequencies in the right of Fig. 3.9a. Both of them are decoupled from the cavity field so that the wavefunction is real and can be interpreted as a condensate wavefunction in position space. The lowest one (a) is proportional to $\sin kx$ in the uniform phase at $\sqrt{N} \eta_l = 15$, having two nodes at $x = 0$ and $\lambda/2$. On increasing the pump strength $\sqrt{N} \eta_l$, the condensate wave function gets more and more localized, hence this excitation contracts into the primary potential well, which is now centered at $x = \lambda/2$ in the self-organized phase. At $\sqrt{N} \eta_l = 120$, the strongly localized BEC feels just the harmonic term of the optical potential. Therefore, at this end, we get for the wavefunction of the excitation something close to the first excitation of a harmonic oscillator. The other selected excitation is the highest one, bending up in Fig. 3.9a. It has six nodes in the homogeneous phase, that corresponds to the third excitation of the Bogoliubov spectrum. It runs side by side with its orthogonal pair up to $\sqrt{N} \eta_l \approx 60$, where they split up. The lower branch tends to the fourth harmonic oscillator excitation in the primary well for $\sqrt{N} \eta_l \rightarrow \infty$, however the upper branch plotted in Fig. 3.10b becomes the first excitation in the secondary well centered at $x = 0$. 
Figure 3.10: The $\delta \psi_+(x)$ components of the eigenvectors of the collective excitations with the lowest (a) and the highest frequencies (b) in Fig. 3.9a are plotted for chosen values of $\eta_t$. In these special cases, the other components are zero.

3.2.5 Summary

In this section, I described the quantum version of the classical self-organization phase transition and gave a detailed account of the steady-state and the dynamics when the atoms form a Bose-Einstein condensate in the cavity. Within the framework of a Gross-Pitaevskii like mean-field model, I showed that the steady-state of the driven condensate is either the homogeneous distribution or a $\lambda$-periodic ordered pattern, and the two regimes are well separated by a critical point. That is, the quantum analogue of the classical phase transition exists for Bose-condensed atoms. The critical point, corresponding to a threshold pump power, has been determined analytically from the Gross-Pitaevskii equation, and also analytically from the spectrum of the excited states. The mean-field results for the self-organization in the classical and in the quantum systems show qualitative agreement. From the expressions of the critical points, one can conclude that in a thermal gas, it is the temperature which stabilizes the homogeneous phase, while in a BEC the same role is played mainly by the atom-atom collisions, and the kinetic energy has only a minor effect. Finally, I studied the spectrum of the collective excitations of the compound BEC-cavity system around the mean-field solution. I found polariton-like excitation modes of the coupled light and matter wave fields. I showed that the spectrum of the collective excitations becomes more intricate in the strong collective coupling regime of cavity QED, where the ordered phase is determined by an asymmetric double well potential with defect sites.
Chapter 4

Excess noise depletion of a Bose-Einstein condensate in an optical cavity

In this chapter, I shall deal with the fluctuations of a Bose-Einstein condensate placed into a single-mode high-finesse optical cavity. In contrast to the transverse pump geometry of the previous chapter, here I consider a BEC–cavity system that is pumped directly through one of the cavity mirrors. Many of the properties of the BEC can be satisfactorily accounted for by assuming a “condensate wavefunction” which obeys a non-linear Schrödinger equation. Nevertheless, atom–atom collisions constantly kick out atoms from the one-particle ground state, even at zero temperature. The atomic population in the excited states of the BEC is called condensate depletion. In a dilute quantum gas, the atom–atom interactions are typically weak, therefore in a BEC the fraction of noncondensed atoms due to s-wave scattering is usually negligible (a few per cent). Large depletion of a BEC can indicate some inherent many-body interaction effect. In case of collisions, such observation requires large local densities. An example is the strong depletion demonstrated as a precursor of the phase transition from superfluid to Mott state in an optical lattice [115, 116]. In this chapter, I will show that a condensate dispersively coupled to the radiation field in a cavity can also be subjected to strong depletion. In this case the many-body effect originates from the long-range atom-atom coupling mediated by the cavity mode, therefore a significant amount of depletion may occur at low density.

A pumped lossy cavity field interacting with a BEC inside is an open system, in which the quantum fluctuations of the radiation field is a possible source of depletion. However, such a fluctuating dipole potential alone cannot imply the unexpectedly large depletion
in the dispersive interaction limit. As it was calculated for a probe field propagating freely through the condensate [117], the depletion scales as the absorption which will be suppressed by choosing very large detuning. Therefore the cavity is essential in creating a specific coupling of the many-atom system to the radiation. Because of the fast round-trips of photons, the cavity field experiences the collective behavior of atoms. This kind of coupling gives rise to the noise amplification mechanism analogous to the so called “excess noise” in laser physics [118, 119, 120, 121].

4.1 Fluctuations around the mean field

In the following, we postulate the mean-field model that is readily discussed in Sec. 2.2.2 and applied in Sec. 3.2. However, we step further by calculating the operator equations of motion of the fluctuations around the mean-field solution, which also includes the quantum noise of the resonator field. This enables one to determine the steady state of the fluctuations, that yields the total number of atoms in the excited states of the condensate.

We consider the one-dimensional motion of ultracold atoms along the axis of a high-Q cavity. A single-mode field, with mode function \( \cos(kx) \), is driven by a coherent laser light through one of the mirrors, and photons leak out at a rate of \( 2\kappa \). The laser frequency \( \omega \) is detuned far from the frequency of the atomic transition \( \omega_A \), i.e., \( |\Delta_A| \gg \gamma \), with the detuning \( \Delta_A \equiv \omega - \omega_A \), and \( 2\gamma \) being the rate of spontaneous emission. Therefore the atom cloud is dispersively coupled to the field, photon absorption by the atoms is neglected. The coupling strength is given by the single-atom phase shift \( U_0 \), where \( U_0 = g^2/\Delta_A \) with \( g \) denoting the single-photon Rabi-frequency in the cavity. The field amplitude operator of the damped-driven mode obeys the standard Heisenberg–Langevin-equation,

\[
i\hbar \frac{\partial}{\partial t} \hat{a}(t) = \left[ -\Delta_C + \int \hat{\Psi}^\dagger(x, t) U(x) \hat{\Psi}(x, t) dx - i\kappa \right] \hat{a}(t) + i\eta + i\hat{\xi}(t),
\]

where \( \Delta_C \equiv \omega - \omega_C \) is the cavity detuning, \( \eta \) is the effective cavity pump amplitude, and the second term including \( U(x) = U_0 \cos^2(kx) \) describes the collective atomic phase shift. The dissipation, given by the \( \kappa \) term, is accompanied by fluctuations which is taken into account by the white noise operator \( \hat{\xi} \). The only non-vanishing correlation function of the noise operator is \( \langle \hat{\xi}(t) \hat{\xi}^\dagger(t') \rangle = 2\kappa \delta(t-t') \). The equation of motion of the atomic field operator is derived from the corresponding dispersive coupling Hamiltonian and reads

\[
i\hbar \frac{\partial}{\partial t} \hat{\Psi}(x, t) = \left[ -\frac{\hbar^2 \Delta}{2m} + \hbar \hat{a}^\dagger(t) \hat{a}(t) U(x) \right] \hat{\Psi}(x, t).
\]
We omit the atom-atom s-wave collision, in order to distil the effects due to the field-mediated coupling between atoms. Note that the two types of interaction involve distinct classes of transitions between the Bloch states of the $\lambda/2$ periodic potential $U(x)$. The atom-photon interaction term is $\lambda/2$ periodic and it does not couple Bloch states with different quasi momenta $q$. We can thus consider wavefunctions being also periodic with $\lambda/2$, the $q = 0$ Bloch state representing the entire band. By contrast, collisions induce transitions mostly within a band. The two types of interaction scale differently with the density and can be treated separately. We consider low densities, where collisions are suppressed and the depletion is due to cavity-induced ‘band-to-band’ transitions. The small amount of additional depletion into higher $q$ states due to s-wave scattering can be independently estimated by the usual formula of the Bogoliubov-theory [106]. The validity of our approach is restricted to parameters where the gas loaded in the cavity lattice field is in the superfluid phase, far from the Mott transition [115, 116].

Following the description presented in Sec. 2.2.2, the field operators are decomposed into mean and fluctuating parts according to

\[ \hat{a}(t) = \alpha(t) + \delta \hat{a}(t), \]  
\[ \hat{\Psi}(x, t) = \sqrt{N} \psi(x, t) + \delta \hat{\Psi}(x, t), \]

with $\alpha(t)$ being the coherent component of the radiation field, and similarly $\psi(x, t)$ stands for the condensate wavefunction normalized to unity, while $N$ is the number of atoms in the condensate. Substituting these into Eqs. (4.1) and neglecting those terms which are not pure c-numbers leads to a coupled pair of nonlinear equations similar in spirit to the Gross-Pitaevskii equations:

\[ i \frac{\partial}{\partial t} \alpha(t) = \left[ -\Delta_C + N \langle U \rangle - i \kappa \right] \alpha(t) + i \eta, \]
\[ i \hbar \frac{\partial}{\partial t} \psi(x, t) = \left[ -\frac{\hbar^2 \Delta}{2m} + \hbar |\alpha(t)|^2 \right] \psi(x, t). \]

The condensate wavefunction $\psi(x)$ couples into the evolution of the field amplitude through the average $\langle U \rangle = \int \psi^*(x, t) U(x) \psi(x, t) \, dx$. The solution of Eqs. (4.3) yields the possible steady-states of the BEC-cavity system.

The Heisenberg-Langevin equations (4.1) can be linearized in the fluctuations $\delta \hat{a}(t)$ and $\delta \hat{\Psi}(x, t)$ around the steady state of Eqs. (4.3). The procedure is similar to that used in Ref. [108] and, for a different geometry in Ref. [92], however, here we will consider the effect of quantum noise. One obtains a coupled set of differential equations for the
fluctuations with couplings to their hermitian adjoints. For a compact notation the fluctuations are arranged in a vector \( \vec{R} \equiv [\delta \hat{a}, \delta \hat{a}^\dagger, \delta \hat{\Psi}(x), \delta \hat{\Psi}^\dagger(x)] \) for which the linearized equation of motion,

\[
i \frac{\partial}{\partial t} \vec{R} = M \vec{R} + i \vec{\xi},
\]

where \( \vec{\xi} = [\xi, \dot{\xi}, 0, 0] \), and the matrix \( M \) is

\[
M = \begin{bmatrix}
A & 0 & \alpha \hat{X}^* & \alpha \hat{X} \\
0 & -A^* & -\alpha^* \hat{X}^* & -\alpha^* \hat{X} \\
\alpha^* Y & \alpha Y & \hat{H}_0 & 0 \\
-\alpha^* Y^* & -\alpha Y^* & 0 & -\hat{H}_0
\end{bmatrix},
\]

with \( A \equiv -\Delta_C + N \langle U \rangle - i \kappa, \ Y \equiv \sqrt{N} \psi(x) U(x), \ \hat{X} f(x) \equiv \int \psi(x) U(x) f(x) dx \) and \( \hat{H}_0 \equiv -\hbar \Delta/(2m) + |\alpha|^2 U(x) \). The key point with respect to the depletion of a BEC is that the matter field fluctuation \( \delta \hat{\Psi}(x) \) couples to both \( \delta \hat{a} \) and \( \delta \hat{a}^\dagger \), this latter being driven by the ‘noise creation’ operator \( \xi \).

The matrix \( M \) has an important symmetry property, namely \( \Gamma M \Gamma = -M^* \), originating from the fact that \( \vec{R}^\dagger = \Gamma \vec{R}^\dagger \), with \( \Gamma \) being the permutation matrix that exchanges the first row with the second and the third row with the fourth one. This property determines the structure of the spectrum. The eigenvalues come in pairs, namely if \( \omega_k \) is an eigenvalue, then \( -\omega_k^* \) will also be an eigenvalue. The other consequence of the above symmetry is that the matrix \( M \) is non-normal, i.e., it doesn’t commute with its hermitian adjoint. Therefore, its eigenvectors are not orthogonal to each other, hence the analogy to excess noise in lasers and to the Peternann-factor arises [122, 123, 124, 125]. The stability can be properly characterized in terms of pseudo-spectra by using the theory of non-normal operators [126, 127]. However, we will restrict this work to the calculation of the depletion of the BEC.

The eigenvalues \( \omega_k \) and the corresponding left and right eigenvectors, \( \ell^{(k)} \) and \( \rho^{(k)} \), respectively, of \( M \) are calculated numerically. First the coupled Gross-Pitaevskii equations (4.3) are solved on a 200 point grid with imaginary time propagation. From the wavefunctions, the matrix \( M \) can be formed and then diagonalized numerically. The spectrum of fluctuations is exhibited in Fig. 4.1, in units of the recoil frequency \( \omega_R = \hbar k^2/m \). The setting \( \kappa = 100 \omega_R \) and the effective number of atoms in the mode \( N = 1000 \) are in accordance with Ref. [86], the other parameters, \( \Delta_C, \eta, \) and \( U_0 \) are rather tunable in practice. At \( U_0 = 0 \), the real part (left panel) renders the spectrum of a homogeneous ideal gas. In a large region \( 0 < |U_0| \lesssim 0.8 \omega_R \) the solid lines corresponding to motional excitations are constant, which indicates that the condensate wavefunction remains close
Figure 4.1: The real and imaginary parts of the eigenvalues of the linear stability matrix $M$ vs. the one atom light shift $U_0$. Only those eigenvalues are plotted which have a nonnegative real part. Every eigenvalue is degenerate at $U_0 = 0$, and the lift of the degeneracy can be resolved only close to $U_0 \approx 1$ for the low-lying levels, where one of the eigenvalue in the quasi-degenerate pair is plotted by thin, dashed line. These are not coupled to the radiation mode and have vanishing imaginary part. The highest plotted eigenvalue at $U_0 = 0$ (thick dashed line) is divided by a factor of 10 and corresponds to a dominantly radiation field excitation; notice that its imaginary part is at $-\kappa$. As $|U_0|$ grows this mode crosses the other excitation energies and reaches zero at $NU_0 \approx \Delta_C$. The parameters are $\Delta_C = -1000 \omega_R$, $\kappa = 100 \omega_R$, $\eta = 1000 \omega_R$, $N = 1000$.

to the homogeneous one. There is a critical point where the condensate pulls the frequency of the cavity mode into resonance with the pump laser frequency ($N \langle U \rangle = \Delta_C$), marked by that the real part of the eigenvalue of the dominantly cavity-type excitation (thick, dashed line) crosses zero. At this point, the steady-state wavefunction is localized in the dipole potential (its depth is about $100 \omega_R$ for the parameters of the figure). Due to the finite spread of the wavefunction around the antinode, the resonance occurs for $U_0$ slightly shifted from $\Delta_C/N$.

Coupling of the motional modes to the radiation mode is signified by the appearance of non-vanishing imaginary parts (Fig. 4.1, right panel). Above the critical point positive imaginary parts appear indicating a dynamical instability of the steady-state solution. This is in accordance with the semiclassical theory of the mechanical forces on atoms in a cavity [63], which states that the cavity field heats up the motion of atoms in the regime of $\Delta_C - N \langle U \rangle > 0$. We will disregard this regime and consider only fluctuations around stable steady-state mean field solutions. Note that the clear maximum of the imaginary
parts reflects the semiclassical result that the cavity cooling mechanism is most efficient at half a linewidth below resonance [67].

4.2 Condensate depletion

Now, we are prepared to solve the linearized equation for the fluctuations Eq. (4.4), and calculate time dependent averages of the form \( C_{ij}(t) = \langle \hat{R}_i(t) \hat{R}_j(t) \rangle \). Especially, we are interested in the steady-state behaviour of the system, when time tends to infinity. As the quantum noise of the cavity continuously excite the collective modes of the coupled light and matter wave fields, there will be a finite steady-state atomic population in the fluctuations.

We carry out the calculation by expanding the fluctuation vector \( \hat{R} \) in terms of “quasi-normal” modes with the help of the left- and right eigenvectors of \( M \) according to \( \hat{R} = \sum_k \hat{\rho}_k \hat{\eta}^{(k)} \). By use of the orthogonality of the left and right eigenvectors, \( \langle \hat{\eta}^{(k)}, \hat{\eta}^{(l)} \rangle = \delta_{k,l} \), where \((a, b)\) is the Euclidean scalar product, the quasi-normal mode amplitude operators are obtained as \( \hat{\rho}_k = \langle \hat{\eta}^{(k)}, \hat{R} \rangle \). They evolve independently

\[
i \frac{\partial}{\partial t} \hat{\rho}_k = \omega_k \hat{\rho}_k + i \hat{Q}_k,
\]

where the projected noise is \( \hat{Q}_k \equiv \langle \hat{\eta}^{(k)}, \hat{\xi} \rangle \). With the integration of Eq. (4.6) the time dependence of the fluctuation operators read

\[
\hat{\rho}_k(t) = e^{-i\omega_k t} \hat{\rho}_k(0) + \int_0^t e^{-i\omega_k (t-t')} \hat{Q}_k(t')dt'.
\]

The depletion is defined as the total population in modes other than the macroscopically populated ground state. It can be expressed in terms of the quasi-normal modes as

\[
\delta N(t) = \int \left\langle \hat{\Phi}^\dagger(x, t) \delta \hat{\Phi}(x, t) \right\rangle dx = \sum_{k,l} \langle \hat{\rho}_k(t) \hat{\rho}_l(t) \rangle \int r_{4k}^2(x) r_{3l}^2(x) dx,
\]

with

\[
\langle \hat{\rho}_k(t) \hat{\rho}_l(t) \rangle = \langle \hat{\rho}_k(0) \hat{\rho}_l(0) \rangle e^{-i(\omega_k + \omega_l)t} + 2\kappa \frac{1 - e^{-i(\omega_k + \omega_l)t}}{i(\omega_k + \omega_l)} l_1^{(k)} l_2^{(l)*}.
\]

By assuming that we start with a pure BEC at \( t = 0 \), the first term is zero. The depletion then reads

\[
\delta N(t) = 2\kappa \sum_{k,l} \frac{1 - e^{-i(\omega_k + \omega_l)t}}{i(\omega_k + \omega_l)} l_1^{(k)} l_2^{(l)*} \int r_{4k}^2(x) r_{3l}^2(x) dx.
\]
Contrary to the case of a conservative system, where quantum depletion is the sum of the individual contributions of the noncondensed one-particle state occupation numbers, here the depletion is the double sum of contributions from pairs of quasi-normal modes \((k\text{ and } l)\).

The denominator in Eq. (4.10) may become small for a pair of eigenvalues \((\omega_k\text{ and } \omega_l)\) if \(\text{Re}\{\omega_k\} = -\text{Re}\{\omega_l\}\), i.e. when the quasi-normal modes \(k\) and \(l\) are connected with the transformation \(\Gamma\). Moreover, the smaller the imaginary parts (their dampings), the smaller the denominator. However, an eigenvalue with a small imaginary part is accompanied by an eigenvector with small “photon” components (diminishing \(l_1\) and \(l_2\) terms). Therefore not all of the eigenvalues with small imaginary parts play a significant role and the evaluation of the terms remains a numerical task. Nevertheless, the contribution to the depletion from such pairs of quasi-normal modes dominates the double sum.

The total steady-state depletion in the \(t \to \infty\) limit (the exponential in Eq. (4.10) is dropped) is shown in Figure 4.2 (semilog scale). The thick solid line corresponds to the parameter set of the spectrum in Fig. 4.1. The depletion is closely constant for a wide range of \(U_0\) up to the resonance regime defined by \(|\Delta_c - N(U)| \lesssim \kappa\). At resonance the depletion diverges, in accordance with the fact that the dynamical equilibrium of the system becomes unstable. It is interesting that there is a dip slightly below the resonance. We attribute it to the significant change in the shape of the condensate wavefunction, from homogeneous to a strongly localized one, which yields a variation of the overlap factors in the matrix \(M\). It is important to note that the finite, large value of depletion in the limit of \(U_0 \to 0\) was calculated by taking first the \(t \to \infty\) limit of the time dependent result Eq. (4.10). However, during a finite measurement time the system does not necessarily reach the steady state since the relaxation time diverges as \(U_0^{-2}\) for small \(U_0\).

It is instructive to approximate the steady-state depletion analytically, since an analytical expression reveals its scaling with the parameters of the system. The studied parameter set is particularly appealing, since for \(0 < |U_0| \lesssim 0.8\omega_R\) the condensate wave function \(\psi(x)\) is practically constant, that is confirmed by the spectrum in Fig. 4.1. The dispersive interaction with the cavity field couples a constant condensate wave function solely to the \(\cos 2kx\) Fourier excitation mode, therefore one can restrict the dynamics into the subspace \(\mathcal{R} = \{\delta \hat{a}, \delta \hat{a}^\dagger, \delta \hat{c}_2, \delta \hat{c}_2^\dagger\}\), where \(\delta \hat{\Psi}(x) = \sqrt{2} \cos 2kx \delta \hat{c}_2\). This procedure resembles the one applied in Sec. 3.2.3, however, in the transverse pumping case the interaction couples the constant condensate wave function to the \(\cos kx\) excitation mode, and below the self-organization threshold the wave function is \textit{exactly} constant. Now,
Figure 4.2: The depletion $\delta N$ of the condensate as a function of the coupling constant $U_0$ for various detunings. The parameters are $\kappa = 100 \omega_R$, $\eta = -\Delta_C$, $N = 1000$, and $\Delta_C = -10^4$, $-10^3$, $-10^2 \omega_R$ for the dashed, solid and dotted lines, respectively. In the plotted range of $U_0$, for smaller detunings (solid and dotted lines) the BEC-cavity system can be resonant with the pump, which leads to divergences. Well below resonance, $N|U_0| \ll \Delta_C$, the depletion depends weakly on $U_0$ (see the plateau of the solid and the dashed lines) and on $N$. In this regime the depletion scales with $\Delta_C/\omega_R$.

in case of cavity pumping, the condensate becomes modulated for any non-zero pump strength, therefore the wave function is only *approximately* constant, thanks to the small interaction strength $U_0$ and the low photon number inside the cavity. The matrix $\mathbf{M}$, defined by Eq. (4.5), then takes the following form in the restricted subspace,

$$
\mathbf{M} = \begin{bmatrix}
A & 0 & \alpha X & \alpha X \\
0 & -A^* & -\alpha^* X & -\alpha^* X \\
\alpha^* Y & \alpha Y & E_2 & 0 \\
-\alpha^* Y & -\alpha Y & 0 & -E_2 
\end{bmatrix},
$$

(4.11)

where the constants appearing in the matrix are $X = \sqrt{2}U_0/4$, $Y = \sqrt{N}U_0/2$ and $E_2 = 4\omega_R + |\alpha|^2U_0/2$. In this simplified model the depletion is $\delta N = \langle \hat{c}_2^\dagger \hat{c}_2 \rangle$, which is calculated by finding the eigenvalues and the corresponding left and right eigenvectors of the matrix $\mathbf{M}$. For the depletion, one gets a similar formula to (4.10), however without the spatial integral over $x$. Skipping the details of the lengthy calculation, the result for
the steady-state depletion is
\[ \delta N \simeq \frac{(\Delta_C - NU_0/2)^2 + \kappa^2}{8\omega_R(-\Delta_C + NU_0/2)}. \] (4.12)

This expression gives a perfect agreement with the numerical results presented in Fig. 4.2 for weak interaction when \( |U_0| \lesssim 0.8 \omega_R \). It explains the slight decrease of the plateaux, which is due to the tuning of the dressed cavity frequency with the collective light shift \( NU_0/2 \) of the homogeneous condensate. Interestingly, the formula accurately describes the resonance of the depletion for \( \Delta_C = -100\omega_R \) (dotted line), giving hyperbolic divergence when the denominator tends to zero. Nevertheless, the restricted model cannot account for the dip and the resonance for \( \Delta_C = -1000\omega_R \) (solid line), since they are located outside the range where the condensate wave function can be taken constant.

The analytical result also yields the order of the steady-state value of the depletion. One can consider two regimes depending on the dressed cavity frequency \( \delta_C = \Delta_C - NU_0/2 \). Typically, the driving field is nearly resonant to the cavity, hence \( \delta_C \) is in the order of \( \kappa \). For instance, setting \( \delta_C = -\kappa \), the magnitude of the depletion becomes \( \delta N = \kappa/(4\omega_R) \). Thus, the number of atoms outside the condensate is simply proportional to the photon loss rate of the cavity. However, in far detuned limit where \( \delta_C \gg \kappa \), the depletion is determined by the ratio of the cavity mode frequency \( \Delta_C \) and the recoil frequency \( \omega_R \), i.e., the relation of the energy scales describing optical excitations and atomic motion, respectively. This is illustrated by the other two curves in Fig. 4.2. Dashed line corresponds to a detuning \( \Delta_C \) increased by an order of magnitude, then the depletion is also scaled up by a factor of 10. Obviously, the resonance regime is pushed out of the plotted range and only the initial plateau can be seen. Oppositely, when decreasing \( \Delta_C \) by a factor of 10, the initial depletion decreases (dotted line). However, for such a small detuning \( \Delta_C \sim \kappa \) the system is in the resonance regime already for small \( U_0 \) values, the wide plateau is missing and the divergence of the depletion is exhibited. As long as the atom-cavity system is far from resonance (on the wide plateau), the depletion \( \delta N \) is independent of the atom number \( N \). Similarly, the photon number \( |\alpha|^2 \) is quite irrelevant to the amount of depletion, it influences only the shape of the ground state in the optical potential and thereby some overlap factors in the matrix \( M \).
4.3 Summary

Quantum fluctuations of a cavity field coupled to the motion of a Bose-Einstein condensate can be strongly amplified by a mechanism analogous to the Petermann excess noise factor in lasers with unstable cavities. For a Bose-Einstein condensate in a stable optical resonator, the excess noise effect amounts to a significant depletion on long timescales. In this chapter, I improved the mean-field description of Sec. 2.2.2 by considering the Heisenberg-Langevin equations for the small fluctuations around the mean-field solution. I determined the spectrum and the normal modes of the polariton-like collective excitations of the system. The atomic population in the fluctuations gives the depletion of the BEC, which I calculated numerically from the solution of the equations of motion. In the weak coupling regime, where the condensate is nearly homogeneous, I approximated the depletion analytically, which shows good agreement with the numerical results. Up to now, we considered the steady-state properties of the system, however, in the next chapter I shall describe the transient dynamics of the fluctuations.
Chapter 5

Nonlinear quantum dynamics of two BEC modes dispersively coupled by an optical cavity

Physics of a coupled BEC-cavity system is interesting in the context of the rapidly developing field of opto-mechanical coupling [128]. Opto-mechanics is ordinarily considered in the context of a cavity system in which the vibrating mirror is coupled to the light field via radiation pressure. In fact, density modulations of the atom cloud amount to effective cavity length changes as does the vibrating mirror. In a recent paper [87], Brennecke et al. have pointed out that the BEC-cavity system in a restricted space of modes can be described by the same, so-called “radiation pressure” Hamiltonian. The interrelation of the parameters in the Hamiltonian, however, are realized in a different regime with a BEC than with a moving mirror. Namely, in the BEC-cavity system the frequency of the mechanical motion, given by the atomic recoil frequency, is well below the dipole coupling strength. By contrast, in the case of a vibrating mirror, its oscillation frequency is on the same order of magnitude as the coupling strength. The other essential difference is that the initial state of the BEC-cavity system is readily the low-excitation quantum regime which, on the other hand, is just the ultimate goal to be reached with mechanical oscillators via various opto-mechanical cooling schemes.

In the following I shall study this quantum regime of the BEC-cavity opto-mechanical system in the low temperature limit. I shall establish the quantum version of the classical model presented in Ref. [87] in the form of a quantum master equation which accounts for non-conservative effects due to the irreversible photon leakage from the cavity. Then, equipped with the consistent description of the pumped-lossy open system, I discuss the
possibility of observing generic quantum effects, such as, for example, the tunneling in an effective double-well potential.

Our model will be based on the two-mode approximation in which atoms from the quasi-homogeneous condensate can be excited only into one other mode, typically into the one with $\cos 2kx$ spatial variation selected by the cavity mode function. This approximation is supported by the analytical result of Chapter 4, which shows that the dominant contribution to the depletion comes from the $\cos 2kx$ BEC excitation mode. Hence, the interaction with the cavity field couples a homogeneous condensate mainly to this specific mode. The two-mode approach is used in several papers together with a semiclassical approximation [87, 129], in which the excited mode is assumed to be in a coherent state with complex amplitude $\phi_2$. Such a simplistic model can explain, for example, the coherent density wave oscillations of a Bose-Einstein condensate observed in recent experiments [87, 95]. We step forward by keeping the excited state mode amplitude as an operator $\hat{\phi}_2$, thereby including quantum statistical effects of the atom cloud.

5.1 The BEC-cavity system and its analogy to optomechanical systems

We consider a zero-temperature Bose-Einstein condensate inside a single-mode high-$Q$ optical cavity. The cavity mode of frequency $\omega_C$ is driven by a coherent laser field of frequency $\omega$. The pump laser frequency is detuned far above the atomic resonance frequency $\omega_A$, so that the atom-pump detuning $\Delta_A = \omega - \omega_A$ far exceeds the rate of spontaneous emission. One can adiabatically eliminate the excited atomic level, and can derive a dispersive atom-field interaction with strength $U_0 = g_0^2/\Delta_A$, where $g_0$ is the single-photon Rabi frequency [63]. We describe the condensate dynamics in one dimension alongside the cavity axis $\hat{x}$, and we assume a single cavity mode function $\cos kx$, with $k = \omega/c$.

We begin with the master equation of the total density operator of the BEC-cavity system,

$$\dot{\rho} = -i [H, \rho] + L \rho . \quad (5.1)$$

The many-particle Hamilton operator in the rotating frame of the pump frequency reads

$$H = -\Delta_C a^\dagger a + i \eta (a^\dagger - a) + \int \Psi^\dagger (x) \left[ -\frac{1}{2\hbar m} \frac{d^2}{dx^2} + U_0 a^\dagger a \cos^2 (kx) \right] \Psi(x) dx , \quad (5.2)$$

where $\Psi(x)$ and $a$ are the annihilation operators of the atom and the cavity fields,
respectively. The parameter $\Delta_C = \omega - \omega_C$ is the cavity detuning, $m$ is the atomic mass. The dissipation is taken into account by the Liouvillian terms

$$\mathcal{L}\rho = \kappa \left( 2 a \rho a^\dagger - a^\dagger a \rho - \rho a^\dagger a \right),$$

(5.3)

with $2\kappa$ being the photon loss rate.

As the coupling term in Eq. (5.2) depends on a cosine function, it is convenient to perform the second quantization of the atom field in the discrete basis of normalized harmonic functions \(\{1, \sqrt{2}\cos nkx, \sqrt{2}\sin nkx\}_{n=1}^\infty\). Since the coupling is \(\cos^2 kx = (1 + \cos 2kx)/2\), just the symmetric modes \(\{1, \sqrt{2}\cos 2nkx\}_{n=1}^\infty\) are involved in the dynamics. The kinetic energy of these modes grows quadratically with the index \(n\): \(E_n = (2n)^2\hbar\omega_R\), where \(\omega_R = h k^2/(2m)\) is the recoil frequency. The energy difference between adjacent modes increases linearly, therefore there is a hierarchy in the respective populations. In the weak-coupling regime, where \(U_0(a^\dagger a) \leq 10\omega_R\), we can approximately restrict the dynamics to the first two modes, i.e. to the constant mode, initially macroscopically populated by the condensate, and to the one that is populated by the interaction with the cavity field in first order. Note that we considered this latter mode in the analytical calculation of the excess noise depletion (Eq. 4.12), which gave good agreement with the numerical results in the weak coupling limit. Accordingly, we write the field operator \(\Psi(x)\) in the form:

$$\Psi(x) = c_0 + \sqrt{2} c_2 \cos 2kx,$$

(5.4)

with \(c_0\) and \(c_2\) being the bosonic annihilation operators of the corresponding modes. In the following, we shall omit the hat from the operators. By inserting this ansatz into Eq. (5.2), we get the following second quantized Hamilton operator:

$$H = \left[ -\Delta_C + \frac{NU_0}{2} \right] a^\dagger a + i\eta (a^\dagger - a) + 4\omega_R c_2^\dagger c_2 + \frac{\sqrt{2}U_0}{4} a^\dagger a \left( c_0^\dagger c_2 + c_2^\dagger c_0 \right).$$

(5.5)

If there is a fixed number of atoms in the two modes \(c_0^\dagger c_0 + c_2^\dagger c_2 = N\), we can consider the atomic system as a macroscopic spin with \(J = N/2\). In this case the Hamiltonian (5.5) is quite similar to the one of the famous Dicke model [130, 131]. However, instead of the Dicke-type coupling term \((a^\dagger + a) J_x\), here the interaction term, \(a^\dagger a J_x\) represents a higher-order nonlinearity.

Having a condensate of a large number of atoms in \(c_0\) together with having a weak interaction, we assume that the condensate ground state is undepleted, and formally set \(c_0 \equiv \sqrt{N}\). Then we end up with the model that describes the coupling between two harmonic oscillators, the driven and lossy cavity mode with amplitude \(a\) and the
amplitude $c_2$ associated with the cos $2kx$ excitation mode of the BEC. By introducing the quadratures (real and imaginary parts) of $c_2$,

$$X = \frac{1}{\sqrt{2}} (c_2^\dagger + c_2) ; \quad Y = \frac{i}{\sqrt{2}} (c_2^\dagger - c_2),$$

the Hamiltonian takes the form

$$H = -\delta_C a^\dagger a + i\eta (a^\dagger - a) + 2\omega_R (X^2 + Y^2) + u a^\dagger a X .$$

Here $\delta_C = \Delta_C - NU_0/2$ is the shifted cavity detuning, and $u = \sqrt{N}U_0/2$, i.e., the single-atom coupling strength $U_0$ is magnified by the square root of the atom number, which can mean several orders of magnitude. Even if the dispersive coupling is very weak due to large detuning, the bosonic enhancement can lead to a significant coupling between the two modes $a$ and $c_2$. The Hamiltonian (5.7) corresponds to the widely studied radiation pressure coupling in opto-mechanical systems [128]. There, in the ordinary opto-mechanical scheme, the cavity photon number is coupled to the position operator of a mirror. Here, in the BEC-cavity system, the $X$ quadrature operator of the atom field excitation mode can be interpreted only as a fictitious 'position'. Although the formal analogy is complete between the two systems, the typical parameters lead to different regimes. In particular, here in the case of the BEC the 'mechanical' vibrational frequency $\omega_R$ is typically much less than other frequencies of the system, which is not the case in usual opto-mechanical setups. Therefore, it is legitimate to make a further approximation for the BEC-cavity system, which consists in using an expansion in terms of the small parameter $\omega_R/\kappa$.

### 5.2 Elimination of the photon field

The Hamiltonian Eq. (5.7) together with the Liouvillean for the cavity mode Eq. (5.3) defines the master equation of the two-mode condensate and cavity system, according to Eq. (5.1). In this section we eliminate the photon field, and incorporate its effects into an effective master equation that accounts for the friction arising from the non-adiabatic response of the cavity field, and for the diffusion stemming from the cavity photon loss noise.

The master equation (5.1) is equivalent with the Heisenberg–Langevin equations

$$\dot{a} = [i(\delta_C - u X) - \kappa] a + \eta + \xi, \quad \dot{X} = 4\omega_R Y, \quad \dot{Y} = -4\omega_R X - u a^\dagger a .$$

(5.8a, 5.8b, 5.8c)
The cavity noise is taken into account by the noise operator $\xi$. It has a vanishing expectation value: $\langle \xi \rangle = 0$, meanwhile its second order correlation is assumed to be a Dirac-$\delta$ function, describing white noise:

$$\langle \xi(t) \xi^\dagger(t') \rangle = 2\kappa \delta(t - t') ,$$  \hspace{1cm} (5.9)

all the other correlations vanish,

$$\langle \xi^\dagger \xi^\dagger \rangle = \langle \xi^\dagger \xi \rangle = \langle \xi \xi \rangle = 0 .$$

### 5.2.1 Adiabatic elimination of the field

On integrating Eq. (5.8a), we get the time dependent solution of the field operator $a(t)$. The time scale of the atomic motion – which we are interested in – is much longer than $1/\kappa$, thus the homogeneous solution with the initial value $a(0)$ vanishes. The particular solution is

$$a(t) = \frac{\eta}{\kappa - i \Delta} + \int_0^t e^{i(\Delta - \kappa)(t-t')}\xi(t')dt' ,$$  \hspace{1cm} (5.10)

where $\Delta \equiv \Delta(X) = \delta_C - uX$. The first term is the steady-state coherent amplitude of the field,

$$\alpha(t) = \eta / (\kappa - i \Delta(X(t))) ,$$  \hspace{1cm} (5.11)

which is now an operator-valued function of the position $X$. The second term in Eq. (5.10) represents an ‘aggregate’ noise, denoted by $\Sigma(t)$. Its expectation value is obviously zero: $\langle \Sigma(t) \rangle = 0$. The second order correlation function can be readily derived from Eq. (5.9),

$$\langle \Sigma(t_1)\Sigma^\dagger(t_2) \rangle = e^{i\delta(t_1-t_2)} \left( e^{-\kappa|t_1-t_2|} - e^{-\kappa(t_1+t_2)} \right) .$$  \hspace{1cm} (5.12)

The ‘aggregate’ noise, having an exponentially decaying correlation function, is a coloured noise with a spectral width $\kappa$. However, on a time scale much longer than $1/\kappa$, the second term in the bracket vanishes, and the remaining part can be approximated by a Dirac-$\delta$ function. Fulfilling proper normalization, the approximate correlation function becomes

$$\langle \Sigma(t_1)\Sigma^\dagger(t_2) \rangle \approx \frac{2\kappa}{\Delta^2 + \kappa^2} \delta(t_1 - t_2) .$$  \hspace{1cm} (5.13)

The dipole force to be substituted into equation (5.8c) is the sum of an adiabatic potential and a noise term:

$$ua^\dagger a = u|\alpha(t)|^2 + \Xi(t) ,$$  \hspace{1cm} (5.14)

with the intensity noise defined as

$$\Xi(t) = u \left( \alpha(t)\Sigma^\dagger(t) + \alpha^\dagger(t)\Sigma(t) + \Sigma^\dagger(t)\Sigma(t) \right) .$$  \hspace{1cm} (5.15)
The noise correlation function is
\[
\langle \Xi(t_1)\Xi(t_2) \rangle = u^2 \langle \alpha^\dagger(t_1)\Sigma(t_1)\alpha(t_2)\Sigma^\dagger(t_2) \rangle = D(X) \delta_\kappa(t_1 - t_2) ,
\]
where the diffusion operator is
\[
D(X) = u^2 |\alpha|^2 \frac{2\kappa}{\Delta^2 + \kappa^2} = u^2 \frac{2\kappa\eta^2}{(\Delta^2(X) + \kappa^2)^2} .
\]
This diffusion process represents the quantum noise transmitted from the photon number fluctuations into the momentum via the optomechanical coupling. We note that here the diffusion is an operator-valued function of the position operator $X$.

### 5.2.2 First-order correction to the adiabatic elimination

When getting the adiabatic field amplitude in Eq. (5.10), the condensate dynamics is assumed to be frozen. This assumption can be relaxed and the atomic motion can be taken into account by means of a systematic expansion in terms of the fictitious momentum $Y$. The small parameter in our model is $\omega_R/\kappa$, because the recovery time of the photon field $1/\kappa$ is small compared to the characteristic time scale of the atomic motion determined by the recoil frequency $\omega_R$. At the same time we will neglect the effect of motion on the fluctuating force $\Sigma$ since it would contribute to the variation of momentum correlation functions in higher orders.

In principle, the field derivative in Eq. (5.8a) can be integrated and the instantaneous field can be obtained from the knowledge of the full “trajectory” $X(t)$. The adiabatic approximation means that the field depends only on the actual position. Close to the adiabatic regime, the history well in the past is irrelevant, and just the local behaviour is important. The trajectory locally can be described by the position and its first derivative, i.e., the momentum. Thus we look for the field amplitude in the form
\[
\alpha(X, t) \cong \alpha_0(X) + \frac{1}{2} \{Y, \alpha_1(X)\} .
\]
where $\{, \}$ denotes anticommutation. We must take care of operator ordering, because $Y$ does not commute with $\alpha_1(X)$. Throughout the calculation we use symmetric ordering.

The time-derivative of a function of an operator, such as $\alpha(X, t)$, is
\[
\frac{d}{dt} \alpha(X, t) = \frac{\partial}{\partial t} \alpha + i [H, \alpha(X, t)] .
\]
In the Hamilton operator of Eq. (5.7), it is only the term $2\omega_R Y^2$ that gives nonzero commutator with $X$. On using that $[Y, \alpha(X)] = -i \frac{\partial \alpha(X, t)}{\partial X}$, one gets
\[
\frac{d}{dt} \alpha(X, t) = \frac{\partial}{\partial t} \alpha + 4\omega_R \frac{1}{2} \left\{ Y, \frac{\partial \alpha(X, t)}{\partial X} \right\} ,
\]
which is symmetrically ordered. Using this derivative on the left-hand-side, and inserting the ansatz Eq. (5.18) to the right-hand-side of Eq. (5.8a), we get a hierarchy of equations in different powers of the operator \( Y \). In zeroth order, we get the adiabatic coherent field amplitude
\[
\alpha_0(X) = \frac{\eta}{-i\Delta(X) + \kappa}.
\] (5.21)
In first order one gets the correction:
\[
\alpha_1(X) = \frac{4\omega_R}{i\Delta - \kappa} \frac{\partial \alpha_0(X)}{\partial X} = i \frac{4\omega_R \eta}{(\kappa - i\Delta(X))^3}.
\] (5.22)
We express the photon number up to first order in \( Y \) with the ansatz Eq. (5.18) as
\[
a^\dagger a = \frac{1}{2}(\alpha \alpha^* + \alpha^* \alpha) = |\alpha_0|^2 + \frac{1}{2} \{Y, \alpha_0^* \alpha_1 + \alpha_0 \alpha_1^*\}. \quad (5.23)
\]
This expansion gives rise to a friction force in the equation of motion of \( Y \) Eq. (5.8c), that is in the form
\[
\mathcal{F}_f = -\frac{1}{2} \{Y, \Gamma(X)\},
\] (5.24)
where the friction coefficient is an operator-valued function of the position operator \( X \):
\[
\Gamma(X) = -16\omega_R u^2 \frac{\Delta(X) \kappa \eta^2}{(\Delta^2(X) + \kappa^2)^3}.
\] (5.25)
Note that damping of the atomic motion is possible via the photon loss channel, if the detuning is a negative-valued function, i.e., \( \langle \Delta(X) \rangle < 0 \), for all states.

### 5.2.3 Effective master equation

Putting the above calculated diffusion (5.14) and friction (5.24) into an effective Heisenberg-Langevin equations, we get the replacement of the Eqs. (5.8b,c), namely,
\[
\dot{X} = 4\omega_R Y,
\] (5.26a)
\[
\dot{Y} = -4\omega_R X - u|\alpha_0(X)|^2 - \frac{1}{2} \{Y, \Gamma(X)\} + \Xi,
\] (5.26b)
Given the effective Heisenberg-Langevin equations, in the next step we can construct an equivalent quantum master equation for the density matrix of the BEC excitation mode,
\[
\dot{\rho} = -i [H_{eff}, \rho] + \mathcal{L}_{diff} \rho + \mathcal{L}_{fric} \rho.
\] (5.27)

Integrating the dipole force in Eq. (5.26b) we get the adiabatic dipole potential which, added to the harmonic oscillator energy, forms the effective Hamilton operator
\[
H_{eff} = 4\omega_R \frac{1}{2} (X^2 + Y^2) + \frac{\eta^2}{\kappa} \arctan \left( \frac{uX - \delta C}{\kappa} \right).
\] (5.28)
It has to be emphasized, that the adiabatic dipole potential is not proportional to the
intensity as in the case of an external laser potential [102]. The reason lies in the back-
action of the atoms on the cavity photon field.

The sum of the harmonic potential and the arcus tangent term can lead to two local
energy minima for certain settings of the parameters. This is the bistability regime and
the effect is closely related to the dispersive optical bistability [83, 132]. Here, the two
minima \((X_c \text{ and } X_h)\) are at opposite sides of the cavity resonance. The one on the cooling
side, \(\Delta(X_c) < 0\), is generally situated farther from the resonance than the one on the
heating side, \(\Delta(X_h) > 0\), i.e., \(|\Delta(X_c)| > |\Delta(X_h)|\). Therefore low photon number and
shallow optical potential correspond to the minimum on the cooling side, accordingly, the
BEC is hardly modulated. Whereas at the heating side minimum, the photon number is
larger, hence the deeper optical potential leads to a more modulated condensate ground
state.

We generalize the standard diffusion and friction terms that appear in the quantum
Brownian motion [133] for position dependent diffusion and friction coefficients. The
momentum diffusion due to the noise source \(\Xi\) can be described by a double commutator
with \(d(X)\),

\[
\mathcal{L}_{\text{diff}} \rho = -[d(X),[d(X),\rho]],
\]

provided the function \(d(X)\) obeys

\[
D(X) = 2 \left( \frac{\partial d(X)}{\partial X} \right)^2.
\]

This differential equation is obtained by matching the variation of the momentum square
mean, \(\langle Y^2 \rangle\) in the Heisenberg-Langevin and in the master equation approaches. After
integration,

\[
d(X) = \frac{\eta}{\sqrt{\kappa}} \arctan \left( \frac{\Delta(X)}{\kappa} \right).
\]

The diffusion can be interpreted as a measurement-induced back-action on the quantum
state of a BEC. The diffusion effect of the field on the BEC has been included in a
master equation for a different scheme where the optical field freely propagates through
the dispersive medium of BEC [117]. In our scheme the measurement can be associated
with the irreversible detection of photons leaking out from the cavity.
Finally, the friction term in Eq. (5.26b) can be reproduced by a term like

$$\mathcal{L}_\text{fric}_\rho = -\frac{i}{2} [g(X), \{Y, \rho\}]$$

(5.32)

in the master equation, provided

$$\Gamma(X) = \frac{\partial}{\partial X} g(X) ,$$

(5.33)

which follows from matching the variation of \langle Y \rangle in the two pictures. The result is

$$g(X) = -\frac{4\omega_R u \kappa \eta^2}{(\Delta^2(X) + \kappa^2)^2} .$$

(5.34)

With this, we have entirely defined the effective master equation (5.27) for the bosonic excitation mode of the BEC. The equation relies on that the ratio \(\omega_R/\kappa\) is small.

5.2.4 Relation with linearized models

Quantum fluctuations in opto-mechanical systems are usually described in models based on linearization: the state of the system is assumed to remain in a small vicinity of a stable stationary solution [134, 135, 136]. Although the master equation (5.27) derived in the previous subsection does not rely on any restriction concerning the range of the variable \(X\), it is instructive to reduce our more general model to the special case where the state of the \(c_2\) mode is well localized around a stationary position \(X_0\) and linearization can be invoked. On the other hand, our model is restricted to small values of \(\omega_R/\kappa\), thus we can make a direct connection to the results of, e.g., the reference [134], provided these latter are expanded up to leading order in \(\omega_R/\kappa\).

Linearization of the master equation can be performed around the energy minimum of the effective Hamiltonian Eq. (5.28). We assume that we are out of the bistable regime, thus, in position representation, the effective potential has a well-defined minimum at \(X_0\). Considering fluctuations around this stationary position,

$$X = X_0 + \delta X ; \quad Y = \delta Y ,$$

(5.35)

the linearized Hamiltonian takes the form:

$$H'_\text{eff} = 2\omega_R (2X_0 \delta X + \delta X^2 + \delta Y^2) + \frac{u \eta^2 \delta X}{(uX_0 - \delta C)^2 + \kappa^2} .$$

(5.36)

In the linearized regime, the optical potential term must have the only effect of shifting the center of the harmonic potential into \(X_0\). As the potential has a minimum at \(X_0\), the
terms linear in $\delta X$ should cancel. Accordingly, we get a self-consistent equation for the equilibrium position:

$$X_0 = -\frac{u}{4\omega_R} \frac{\eta^2}{(uX_0 - \delta_C)^2 + \kappa^2}. \quad (5.37)$$

Outside the bistable regime, this third order equation has only one real solution. If $|uX_0| \ll \kappa, \delta_C$, then an approximate value of $X_0$ can be obtained by neglecting the $X_0^3$ dependence of the denominator on the right hand side. Linearization of the diffusion and friction terms is readily available from Eq. (5.30) and Eq. (5.33), thus

$$d(X) = d(X_0) + \sqrt{\frac{D(X_0)}{2}} \delta X, \quad (5.38)$$

$$g(X) = g(X_0) + \Gamma(X_0) \delta X. \quad (5.39)$$

The constant terms drop from the commutators, and we recover the famous Caldeira-Legett master equation [137] with diffusion and friction coefficients depending on the stationary position $X_0$:

$$\dot{\rho} = -i \left[ H_{\text{eff}}, \rho \right] - \frac{D(X_0)}{2} [\delta X, [\delta X, \rho]] - \frac{i}{2} \Gamma(X_0) [\delta X, \{\delta Y, \rho\}]. \quad (5.40)$$

Note that after the linearization, the diffusion and the friction are no longer described by operators, but by real numbers. Hence, we can easily express the steady-state excitation number of the oscillator:

$$\bar{n}(X_0) = \frac{D(X_0)}{\Gamma(X_0)} = -\frac{\Delta^2(X_0) + \kappa^2}{8\omega_R \Delta(X_0)}. \quad (5.41)$$

Let us analyze the weak coupling limit, where $|uX_0| \ll \kappa, \delta_C$, and one can neglect the $X_0^3$-dependence of the cavity detuning, thus $\Delta(X_0) \approx \delta_C = \Delta_C - NU_0/2$. In this case, the expression Eq. (5.41) simplifies to

$$\bar{n} = \frac{(\Delta_C - NU_0/2)^2 + \kappa^2}{8\omega_R (-\Delta_C + NU_0/2)}. \quad (5.42)$$

This agrees with Eq. (6) of Ref. [134], by using the correspondence between the notations, $\omega_m \rightarrow 4\omega_R$, $4\tau^2 \rightarrow 1/\kappa^2$, $\Delta_L \rightarrow \delta_C$. Let us also note, that for a BEC, the excitation number of the “oscillator” corresponds to the population in the $e_2$ mode, that is nothing else but the condensate depletion already calculated in Chapter 4. The steady-state excitation number of the oscillator Eq. (5.42), which we obtained from the linearized master equation, is equal to the condensate depletion Eq. (4.12) derived in the weak coupling limit.
We can deduce the criterion of linearization, since the mean excitation number determines the magnitude of the fluctuations $\delta X$, as $\bar{n} = \langle \delta X^2 \rangle / 2$. The small parameter in the Taylor-series expansion of the arcus tangent function was

$$
\delta X \frac{u}{\kappa} \left[ 1 + \left( \frac{\Delta(X_0)}{\kappa} \right)^2 \right]^{-1} \ll 1.
$$

(5.43)

Raising the expression to second power, taking the average and replacing $\langle \delta X^2 \rangle$ by Eq. (5.41), one gets a restriction to the strength of the atom-field interaction:

$$
u^2 \ll 8 \omega_R |\Delta(X_0)| \left[ 1 + \left( \frac{\Delta(X_0)}{\kappa} \right)^2 \right].
$$

(5.44)

The effective cavity detuning $\Delta(X_0)$ needs to be in the order of the cavity decay rate $\kappa$ for the cavity to have considerable effects, hence the condition of linearization becomes, roughly, $\nu^2 \ll 8 \kappa \omega_R$.

### 5.3 Tunneling in the optical bistability regime

In the effective Hamiltonian (5.28), the arcus tangent term added to the harmonic potential may lead to two minima, i.e., to a kind of double-well potential [138], for certain parameter settings. Classically, this regime corresponds to bistability [139, 87]. There are two distinct equilibrium states of the excited mode $c_2$, c.f., the third-order algebraic equation (5.37) has two real solutions. Our objective in this section is to study the dynamics of the quantum system in this regime. In particular, we are interested in the eventual quantum interference of the distinct mean-field solutions.

Let us analyse the spectrum of the effective Hamilton operator of Eq. (5.28) in the bistability regime. The lowest energy levels are plotted in Fig. 5.1a as a function of the effective cavity detuning $\delta_C$. For the parameters of the figure, the range of bistability is $\delta_C = -920.7 \ldots -773.5 \omega_R$. The harmonic oscillator spectrum is considerably modified by the optical dipole potential of the cavity field. The arcus tangent type potential inherits the resonant character of the field. Far from the resonance, where the argument of the arcus tangent is large, it gives just a $\pm \pi \eta^2/2 \omega_R$ energy shift to the equidistant energy levels of a harmonic oscillator of frequency $4 \omega_R$. Around the resonance, the optical potential alters the level structure of the oscillator more significantly: (i) it reduces the distance between the neighboring levels, and (ii) it gives rise to avoided crossings, e.g., between the two lowest energy levels at $\delta_C \approx -825 \omega_R$ (see the inset). For better visibility of the alteration...
of the distance between adjacent levels, these energy differences are plotted in Fig. 5.1b. On the left most and right most sides, the differences tend to $4\omega_R$, i.e., back to the level spacing of the harmonic oscillator (the convergence on the right most side cannot be seen in the plotted range). There is a significant dip at the bistable regime. A dip approaching zero would mean two minima separated by a very high barrier. In the different eigenstates $\phi_n$ the resonance of the filled cavity, determined by $\langle \phi_n | \Delta(X) | \phi_n \rangle = 0$, is at different frequencies, thus the dips are shifted from level to level.

Consider now the two lowest energy levels in the minimum of the dip at $\delta_C = -825\omega_R$. The corresponding wave functions are plotted on the left of Fig. 5.2, the ground state $|\phi_0\rangle$ (solid red) and the first excited state $|\phi_1\rangle$ (dashed green). The figure shows the marked difference with respect to the displaced eigenstates of a harmonic oscillator. The ground state, for example, is two-peaked, reflecting the effect of a potential barrier in its center. Note, that due to the “optical force” both wave functions are shifted towards a range with negative $X$ values ($X = 0$ would be the center of the harmonic potential). As usual in the case of a double well potential, the symmetric and antisymmetric combinations of the two lowest energy eigenstates,

$$|r\rangle = \frac{1}{\sqrt{2}}(|\phi_0\rangle + |\phi_1\rangle) \quad \text{and} \quad |l\rangle = \frac{1}{\sqrt{2}}(|\phi_0\rangle - |\phi_1\rangle),$$

(5.45)

can be considered as ‘localized’ wave functions in the left and right potential wells. These states could be associated with the classical equilibrium solutions, however, as the plot on the right of Fig. 5.2 shows, they noticeably penetrate into the other well for the given value of $\Delta_C$. If we start the system from the left state $|\Psi(0)\rangle = |l\rangle$, then, by inserting
Figure 5.2: Left: The wave functions of the ground state and of the first oscillator excitation. Right: The symmetric and antisymmetric combination of the two (left and right states) defined in Eq. (5.45). Parameters: $\delta_C = -825 \omega_R$, $u = 169.74 \omega_R$, $\kappa = 342.1 \omega_R$, $\eta = 120 \omega_R$.

the time evolution of the energy eigenstates, we get

$$|\Psi(t)\rangle = \frac{e^{-i\omega_0 t}}{\sqrt{2}}(|\phi_0\rangle + e^{-i(\omega_1 - \omega_0)t}|\phi_1\rangle).$$

(5.46)

Hence, the system in this superposition oscillates between $|r\rangle$ and $|l\rangle$ with the frequency that corresponds to the energy difference $\omega_{10} = \omega_1 - \omega_0 = (E_1 - E_0)/\hbar$. In fact, this is true also for a harmonic oscillator with its own frequency. The slowing down of the oscillations between left and right is the signature of a barrier. These oscillations realize tunneling only if the barrier height is superior to the energy of the quantum state. In our case the energy of the higher lying level is $E_1 = 49.45 \hbar \omega_R$, that is just below the height of the barrier $E_b = 49.52 \hbar \omega_R$, and the bottoms of the potential wells lie at 48.0 and 47.8 $\hbar \omega_R$.

Calculating the expectation value of the position operator $X$ in the state $|\Psi(t)\rangle$, we get an oscillation

$$\langle \Psi(t) | X | \Psi(t) \rangle = \frac{1}{2} (X_{00} + X_{11}) + X_{01} \cos \omega_{10} t,$$

(5.47)

with $X_{nm} = \langle \phi_n | X | \phi_m \rangle$. The amplitude of the coherent oscillation is given by $X_{01}$. We find maximum tunneling by plotting this off-diagonal matrix element of the position operator $X_{01}$ as a function of the effective cavity detuning in Fig. 5.3. The oscillation amplitude $X_{01}$ shows a resonant character (c.f. resonant tunneling). For large positive or negative detunings, the cavity field is practically zero, and we get the matrix element $X_{01}^{HO} = 1/\sqrt{2}$ for the harmonic oscillator to which the plotted curve is normalized. There is a sharp peak indicating the detuning where the largest population oscillates between
the two wells. The position of the peak is \( \delta_C = -825 \omega_R \), that coincides with the point where the energy difference between the two states is the smallest (compare to Fig. 5.1).

The expectation value of the position operator \( \langle X \rangle(t) \) assuming coherent time evolution of the system from the initial left state \(|l\rangle\) is plotted in Fig. 5.4 with dashed green curve. We set \( \delta_C = -825 \), where the amplitude of the coherent oscillation is maximum (c.f. Fig. 5.3) with \( X_{01} = 1.6 \), and its frequency is given by the minimum energy difference between the ground state and the first excited state (red curve in Fig. 5.1b), i.e. \( \omega_t = 0.63 \omega_R \). The dashed green curve nicely reproduces the expected result of Eq. (5.47). However, when diffusion and friction are taken into account, the time evolution of \( \langle X \rangle(t) \) exhibits a significantly different result, plotted with solid red line in the figure. We simulated numerically the full master equation (5.27) on the harmonic oscillator basis truncated at the lowest 300 eigenstates. We found that the diffusion rate is nearly ten times larger than the tunneling rate, therefore it inevitably destroys the superposition of the two energy eigenstates before the first ‘round-trip’ is completed. The mode is excited to the higher lying energy eigenstates, being unaffected by the dipole potential and thus the mean \( \langle X \rangle(t) \) tends to zero on the long run. In the initial transient, however, oscillations appear with the frequency \( \omega \approx 3.4 \omega_R \), that is close to the oscillator’s own frequency \( 4 \omega_R \). These oscillations are produced by the higher energy states, to which the diffusion scattered out the initial state. For completion we plot the time
Figure 5.4: Expectation value of the position operator during the time evolution of the total system started from the $|l\rangle$ (solid red) and $|r\rangle$ (dotted blue) states. For the former case the dynamics without the friction and diffusion terms is also plotted (dashed green). Parameters: $\delta_C = -825 \omega_R$, $u = 169.74 \omega_R$, $\kappa = 342.1 \omega_R$, $\eta = 120 \omega_R$.

The evolution of $\langle X \rangle$ when starting the system from the ‘right’ state $|r\rangle$ with dotted blue line. In this case, the dephasing effect is more conspicuous, as the transient oscillations are smaller.

In the end of this section, let us show that the diffusion is generally larger than the tunneling rate in the bistability range. There is a critical pumping strength $\eta_c^2 = \frac{32}{3\sqrt{3}} \frac{\kappa \omega_R}{u^2}$ above which bistability occurs [95]. It imposes a lower bound on the diffusion operator of Eq. (5.17), that is $D_L(X) = \frac{64}{3\sqrt{3}} \frac{\omega_R^2}{\langle \Delta(X)^2 + \kappa^2 \rangle} \omega_R$. Interestingly, its order of magnitude is given by a constant, $\frac{64}{3\sqrt{3}} \omega_R \approx 12 \omega_R$. The tunneling rate, however, has an upper limit, that is the frequency of the oscillator $4 \omega_R$. With a pumping strength being in the order of the bistability threshold, $\eta \approx \eta_c$, a tunneling rate of $\omega_R$ can be achieved. The diffusion operator should be averaged over a time-dependent tunneling state. Nevertheless, the average of $\frac{\kappa^2}{\langle \Delta(X)^2 + \kappa^2 \rangle^2}$ is expected to be around unity, because the right and left sites are situated on the opposite sides of the resonance, and for $\eta \approx \eta_c$ they are close to each other. By increasing the pumping strength far above $\eta_c$, the average of the diffusion slightly decreases, while the tunneling rate drops dramatically. Hence, the diffusion is at least one order of magnitude larger, than the tunneling rate, therefore it impedes the observation of quantum tunneling in the double-well potential.


5.4 Coherent density wave oscillations

By contrast to the previous example of considering the lowest lying energy states as the initial state, here we will calculate the evolution from an initially highly excited, coherent wave packet. To this end, we numerically solved the effective master equation (5.27) for the $c_2$ mode on the basis of the harmonic oscillator Fock states up to 400.

Figure 5.5: Hamiltonian dynamics (with Eq. (5.28)) of the system started from an initial coherent state with coherent amplitude $c_2 = 7/\sqrt{2}$. (a) Expectation value (solid blue) and variance (dotted brown) of the position operator. The dashed red line shows the position of the cavity resonance. (b) Intracavity field intensity. Parameters: $\delta_C = -825\omega_R$, $u = 169.74\omega_R$, $\kappa = 342.1\omega_R$, $\eta = 120\omega_R$.

Figure 5.6: Solution of the master equation (5.27). (a) Expectation value (solid blue) and variance (dotted brown) of the position operator. The dashed red line shows the cavity resonance. (b) Intracavity field intensity. Parameters: $\delta_C = -825\omega_R$, $u = 169.74\omega_R$, $\kappa = 342.1\omega_R$, $\eta = 120\omega_R$. 

\[c_2^2 = \frac{7}{\sqrt{2}}\]
As a reference, we plot the time evolution of the system without cavity noise and friction. For initial condition, a coherent state is set with coherent amplitude $c_2 = 7/\sqrt{2}$. In Fig. 5.5a we show the mean value (solid blue) and the variance (dotted brown) of the position operator. The corresponding intracavity photon number is shown in Fig. 5.5b. The mean value reflects the coherent oscillations in the confining potential. The intracavity field intensity depends on $X$, according to Eq. (5.21), hence peaks appear in the photon number (Fig. 5.5b) in each oscillation period of $X$, when $\langle X \rangle$ crosses cavity resonance at the value of $-4.9$ (dashed red). Even in the pure Hamiltonian dynamics, the visibility of the oscillations gets reduced as time goes on. The reason is the diffraction of the wave packet on the central hump of the double well potential, which is represented by the growing variance of $X$ in the figure. As the wave packet spreads, its motion cannot be resolved with the cavity linewidth, and the double peak structure vanishes after $3\tau_R$.

The evolution of the full master equation gives qualitatively similar results, see Fig. 5.6, however due to the diffusion the spread of the quantum state increases faster, indicated by the increase in the variance of the position operator (dotted brown). Hence, we get larger decay for the oscillation of $\langle X \rangle$ (solid blue), and for the corresponding decay of the photon peaks (b). It is important to note, that the origin of the decay is not the friction but the diffusion. In fact, at this set of parameters the friction, being a correction of order $\omega_R/\kappa$, is negligible and we see a pure dephasing effect due to diffusion. In this nonlinear dynamics the decay is far from being exponential, therefore it cannot be described by a single decay rate, rather the decay rate changes in time. In Fig. 5.6a the decay of $\langle X \rangle$ is more remarkable in the beginning of the oscillation, while the decay slows down after $3\tau_R$. The diffusion is large during the photon peaks, when the cavity is in resonance with the pumping laser. The resonance condition $\langle \Delta(X) \rangle = 0$ is fulfilled at $\langle X \rangle = -4.9$, therefore most of the diffusion takes place, when $\langle X \rangle$ crosses this resonance line (dashed red). This explains the slowing down of the decay. After $3\tau_R$, the full oscillation is above the resonance line, so the photon peaks drop down, as well as the diffusion.

The average diffusion also depends on the amplitude of the coherent oscillation. For larger amplitudes the `velocity’ $(\partial X/\partial t)$ is larger, as the oscillation frequency is nearly the same. Thus, the system spends less time in the vicinity of the cavity resonance, which means that the photon peaks become narrower in time, hence the average diffusion decreases. To demonstrate this, we plot $\langle X \rangle(t)$ for a system started with coherent amplitudes $5/\sqrt{2}$ and $10/\sqrt{2}$ in Fig. 5.7. The two curves are shifted to the center and normalized by the corresponding oscillation amplitudes. One can observe that the frequency
is slightly larger (closer to $4\omega_R$) for larger amplitude oscillations, however the important observation is that the decay is significantly reduced when the system is started from a larger coherent amplitude. This explains why the experiment [87] could produce well resolved double peaks. The initial coherent amplitude was so large that the system was far from resonance most of the time, and thus, in the lack of cavity photons, the diffusion is effectively suppressed.

### 5.5 Summary

In this chapter I studied the interaction of a Bose-Einstein condensate and a single-mode optical cavity in a full quantum model. In the weak coupling limit, the cavity mode appoints a single condensate excitation mode that dominantly couples to the cavity field. Keeping only this single excitation mode, the BEC-cavity system becomes formally analogous to a class of opto-mechanical systems. By eliminating the photon field, I derived a quantum master equation for the BEC excitation mode playing the role of the mechanical oscillator. Adiabatic elimination of the field led to an effective optical potential in the master equation that has been showed to produce optical bistability. Dissipation of the cavity field is taken into account by diffusion and friction terms, with friction being determined as the first order correction to the adiabatic elimination in the small parameter $\omega_R/\kappa$. Linearization of the master equation establishes a connection with linearized
models describing vibrating mirrors in the literature, and it enabled us to calculate analytically an equilibrium excitation number in the extra weak coupling limit. Using the effective master equation, I simulated the nonlinear quantum dynamics of the BEC excitation in the bistability regime. I generally showed that quantum tunneling is hindered by the dephasing process accompanied by photon loss. Nevertheless, coherent matter wave oscillations are possible, where diffusion is less dominant for larger amplitude oscillations.
Chapter 6

Dipole-dipole instability of atom clouds in a far-detuned optical dipole trap

In this chapter, I consider the radiative interaction between cold atoms trapped inside a far-off-resonance dipole trap (FORT). Although this work is somewhat lateral to the main body of the Thesis, it provides a complement to the models used in the previous chapters, since it allows for treating an effect which is usually omitted from the description. The light-induced dipole-dipole interaction between the atoms in a laser field has indeed a small effect at typical atom densities and laser powers, however, it is instructive to calculate the limit above which this type of atom–atom interaction becomes significant.

In dense samples of cold atoms, two-atom processes strongly influence the trapping. For example, collisional processes (photo-association, hyperfine ground state changing collisions) are known to result in trap losses and they can limit the maximum achievable density. Collisions usually depend heavily on the internal electronic structure of the species. For interatomic distances in the range of the optical wavelength, the atom-atom interaction is dominated by the radiative electromagnetic coupling. In this case one can distinguish two limits: the photon scattering is dominated (i) by spontaneous emission, e.g. in magneto-optical traps (MOT), and (ii) by stimulated emission, which occurs in far-off-resonant dipole traps (FORT). Since the MOT enabled us first to capture dense atom clouds from vapour, it was first analyzed with respect to radiative many-body effects [23, 140]. In a MOT, the cooling laser is quasi-resonant with the atoms and the sample forms an optically thick medium. The depletion of the laser beams together with the multiple spontaneous scattering of resonant photons within the sample can lead to instability [23] and extra heating [141, 142]. At high densities, the reabsorption of photons influences the laser cooling itself [143, 144]. The combination of these effects can result
in a highly nonlinear collective dynamics of the atom cloud in a MOT [145, 146].

The FORT operates at an extremely low spontaneous scattering rate, thus the effects of multiple spontaneous photon scattering are strongly suppressed. The mechanism of trapping relies on the process of absorption and stimulated emission of laser photons. This process polarizes the particles, hence the dipole force is accompanied by the dipole-dipole coupling between atoms. In previous works a phenomenological term proportional to the square of the atom density was introduced to describe the atom-atom interaction, e.g., the effect of collisions on the loading of a FORT [147, 148]. This dominates in strongly localized traps, collisional blockade can prevent us from confining even two atoms in an extremely tiny FORT [149].

High atom densities can be an issue for many kinds of experiments with FORT's. One example is the attempt to achieve Bose-Einstein condensation with alkali gases in optical rather than magnetic traps [150, 151]. The stability of an atom cloud against dipole-dipole coupling is an issue also in the ultracold temperature regime where the atoms form a degenerate Bose-condensate. The corresponding anisotropic potential can be included in the Gross-Pitaevski equation [152]. There is a stable solution for the atomic mean-field wavefunction depending on the trap aspect ratio [153], or on the scattering length [154, 155]. The dipole-dipole interaction gives rise to density modulations [156], solitons [157]. In these works the atoms possess a permanent dipole moment. Recently, the effects of the magnetic dipole-dipole coupling has been observed in a chromium condensate [158]. The laser induced dipole-dipole coupling at low temperatures has been treated in [159] and was shown to lead to nonlinear atom optical effects. An interesting question arises that whether the dipole-dipole interaction excludes the possibility of forming a Bose-Einstein condensate in an optical dipole trap.

6.1 Dipole-dipole interaction

The theory of radiative atom-atom interaction in the presence of a driving laser field is described in several papers, e.g. Refs. [144, 159, 160, 161], we will mostly use the approach presented in [161].

We consider a number $N$ of atoms interacting with a single Gaussian standing-wave laser field mode along the $\hat{z}$ direction which has a mode function

$$f(r) = \xi \cos(k_L z) \exp \left[ -2\pi^2 (x^2 + y^2)/w^2 \right],$$  \hspace{1cm} (6.1)

where $\xi$ is the field polarization, and the mode is paraxial, $k_L \gg 2\pi/w$. The atomic
transition frequency is $\omega_A$, that of the laser field mode is $\omega_L$, and the detuning is defined by $\Delta_A = \omega_L - \omega_A$. The atom-mode interaction strength is described by the Rabi frequency $\Omega$ in the position of maximum coupling. We assume an $S \leftrightarrow P$ transition with a degenerate manifold of excited states and keep the three-dimensional polarizability of the atoms. Actually the fixed field polarization selects two levels taking part in the dynamics. The atomic internal degree of freedom is described by the vectorial lowering operator $\sigma = \sum_q \varepsilon_q \sigma_q$ with $q = \pm 1$ and $q = 0$ corresponding to the circular and linear polarizations, respectively. The quantization axis will be defined in accordance with the choice of the field polarization $\varepsilon_q$.

The equation of motion for the density operator in the Markov approximation reads

$$\dot{\rho} = \frac{1}{i\hbar}[H, \rho] + \mathcal{L}\rho.$$  \hfill (6.2)

In a frame rotating at the laser frequency $\omega_L$, the Hamiltonian is

$$H = \sum_{n=1}^N \left[ \frac{\mathbf{p}_n^2}{2m} - \hbar \Delta_A \sigma_n^+ \sigma_n - i\hbar \Omega \int (\varepsilon_n) \left( \sigma_n^+ - \sigma_n \right) \right] - \hbar \gamma \sum_{n,m=1}^N \sigma_n^+ \beta(R_{nm}) \sigma_m,$$  \hfill (6.3)

where $\varepsilon_n$, $\mathbf{p}_n$, and $\sigma_n$ are the position, the momentum and the polarization of the $n$th atom ($n = 1, \ldots, N$). Next to the single atom terms, i.e. kinetic energy, internal energy, and atom-field coupling, the last term contains the induced dipole-dipole interaction energy of the atoms. Note that the natural linewidth $\gamma$ characterizes the strength of this interaction. The tensor $\beta$ depends on the coordinate difference $R_{mn} \equiv \varepsilon_n - \varepsilon_m$ of the interacting pairs of atoms.

The dipole-dipole interaction is mediated by the broadband vacuum, and is therefore accompanied by incoherent evolution. This is represented by additional terms in the Liouville operator responsible for the dissipation:

$$\mathcal{L}\rho = -\gamma \sum_{n=1}^N \left( \{ \sigma_n^+, \sigma_n, \rho \} - 2 \sum_q \int d^2 \mathbf{u} N_q(\mathbf{u}) \sigma_n^q e^{-ik_{q,\mathbf{u}} R_{nn}^q} \rho e^{ik_{q,\mathbf{u}} R_{nn}^q} \sigma_n^q \right)$$

$$- \gamma \sum_{n,m=1}^N \sum_{n \neq m} \left( \{ \sigma_n^+, \alpha(R_{mn}) \sigma_n, \rho \} - 2 \int d^2 \mathbf{u} \sigma_n N(\mathbf{u}) e^{-ik_{n,\mathbf{u}} R_{nn}} \rho e^{ik_{n,\mathbf{u}} R_{nn}} \sigma_n^+ \right),$$  \hfill (6.4)

where $\{ , \}$ denotes the anticommutator. The single atom terms include the spontaneous decay accompanied by momentum recoil. The tensor $N(\mathbf{u}) = \frac{3\gamma}{8\pi}(1 - \mathbf{u} \cdot \mathbf{u})$, and its diagonal elements $N_q(\mathbf{u}) = \varepsilon_q N(\mathbf{u}) \varepsilon_q$ are the angular momentum distribution of the spontaneous emission from the $q$-state in the excited manifold. Here $1$ is the two-by-two
unit matrix, and $\odot$ denotes dyadic product. The double sum describes the loss effect due to the dipole-dipole coupling.

In free space the tensors $\alpha$ and $\beta$ assume the following form:

$$\alpha(R_{mn}) = \frac{3}{2} \left\{ (1 - \hat{R}_{mn} \odot \hat{R}_{mn}) \frac{\sin kR_{mn}}{kR_{mn}} + (1 - 3\hat{R}_{mn} \odot \hat{R}_{mn}) \left( \frac{\cos kR_{mn}}{(kR_{mn})^2} - \frac{\sin kR_{mn}}{(kR_{mn})^3} \right) \right\}, \quad (6.5)$$

$$\beta(R_{mn}) = \frac{3}{2} \left\{ (1 - \hat{R}_{mn} \odot \hat{R}_{mn}) \frac{\cos kR_{mn}}{kR_{mn}} - (1 - 3\hat{R}_{mn} \odot \hat{R}_{mn}) \left( \frac{\sin kR_{mn}}{(kR_{mn})^2} + \frac{\cos kR_{mn}}{(kR_{mn})^3} \right) \right\}, \quad (6.6)$$

where $k = |k| \approx k_L$, $R_{mn} = |R_{mn}|$, and $\hat{R}_{mn}$ is a unit vector along the direction of $R_{mn}$.

The fixed field polarization selects the excited state and the atom reduces to a two-level system with $\sigma_n = \sigma_n \xi (n = 1, \ldots, N)$. The tensors $\alpha$ and $\beta$ have to be projected onto this particular polarization,

$$\sigma_m^\dagger \beta(R_{mn}) \sigma_n = \beta(R_{mn}) \sigma_m^\dagger \sigma_n, \quad (6.7)$$

where $\beta(R_{mn}) = \xi^\dagger \beta(R_{mn}) \xi$. We now evaluate this projection in two cases: for linear polarization along $\hat{x}$, and for circular one in the $\hat{x}$-$\hat{y}$ plane.

### 6.1.1 Linear polarization

When the polarization of the beam is linear, $\xi = \hat{x}$, the atomic quantization axis is taken in this direction. The atomic polarization is described by the operator $\sigma_0$, and the projection given in Eq. (6.7) results in

$$\beta_{mn} = \frac{3}{2} (3 \cos^2 \phi_{mn} - 1) \left[ \frac{\sin kR_{mn}}{(kR_{mn})^2} + \frac{\cos kR_{mn}}{(kR_{mn})^3} \right] + \frac{3}{2} (1 - \cos^2 \phi_{mn}) \frac{\cos kR_{mn}}{kR_{mn}}, \quad (6.8)$$

where $\phi_{mn} = \angle(R_{mn}, \hat{x})$ is the angle between the distance vector of the two atoms and the axis of the polarization, $\hat{x}$. As this function is singular at the origin, $kR_{mn} \to 0$, later we will use rather its Fourier transform [162],

$$\tilde{\beta}(k) = \lim_{\eta \to 0} \frac{3}{\sqrt{2\pi k_L^3}} \frac{(k_L^2 + k_n^2)(k^2 - k_L^2 + \eta^2)}{k^2 - k_L^2 + 2\eta^2(k^2 + k_L^2)} \quad (6.9)$$
6.1.2 Circular polarization

If the polarization is circular, \( \xi = -\frac{i}{\sqrt{2}}(\hat{x} + i\hat{y}) \), the atomic quantization axis is the field propagation direction \( \hat{z} \). The atomic polarization is described by the operator \( \sigma^+ \), and the projection Eq. (6.7) gives

\[
\beta_{mn} = \frac{3}{4} (1 - 3 \cos^2 \theta_{mn}) \left[ \sin \frac{kR_{mn}}{(kR_{mn})^2} + \cos \frac{kR_{mn}}{(kR_{mn})^3} \right] + \frac{3}{4} (\cos^2 \theta_{mn} + 1) \frac{\cos kR_{mn}}{kR_{mn}}. \tag{6.10}
\]

The angle \( \theta_{mn} = \angle(\mathbf{r}_{mn}, \hat{z}) \) is the angle between the distance vector of the two atoms and the axis \( \hat{z} \). The Fourier transform is

\[
\tilde{\beta}(k) = \lim_{n \to 0} \frac{3}{2\sqrt{2\pi k^3}} \frac{(k^2 + k^2)(k^2 - k_L^2 + \eta^2)}{(k^2 - k_L^2)^2 + 2\eta^2(k^2 + k_L^2)}.
\tag{6.11}
\]

6.2 Large detuning limit

For red detuning (\( \Delta_A < 0 \)) the atoms are attracted to high-intensity regions of the field. In the large detuning limit, i.e., where the magnitude of \( \Delta_A \) exceeds the atomic linewidth \( \gamma \) by far, \( |\Delta_A| \gg \gamma \), the laser field creates a conservative potential for the atoms. The recoil noise is so strongly suppressed that heating plays no role on the relevant timescale of motion. It is enough to consider only the conservative part of the dynamics described by the Hamiltonian. The dissipative processes will be taken into account later by the introduction of a phenomenological temperature.

The internal electronic dynamics of the atoms consists of fast oscillations on a short timescale. This can be adiabatically eliminated to derive its effect on the external motion. The adiabatic atomic polarizations, derived from the equations of motion according to Eq. (6.3), obey the implicit equation

\[
\sigma_n = \frac{\Omega}{\Delta_A} f(\mathcal{L}_n) + \frac{\gamma}{\Delta_A} \sum_{m \neq n}^N (\alpha_{mn} - i\beta_{mn}) \sigma_m.
\tag{6.12}
\]

To leading order in \( |\gamma/\Delta_A| \), the polarization is just the first term, which gives the zeroth order of the Hamiltonian:

\[
H_{\text{eff}}^{(0)} = \sum_{n=1}^N \left( \frac{p_n^2}{2m} + \frac{\hbar \Omega^2}{\Delta_A} f^2(\mathcal{L}_n) \right) - \frac{\hbar \gamma \Omega^2}{\Delta_A^2} \sum_{n,m}^N \beta(\mathcal{L}_n - \mathcal{L}_m) f(\mathcal{L}_n) f(\mathcal{L}_m). \tag{6.13}
\]

This Hamiltonian \( H_{\text{eff}}^{(0)} \) describes the dynamics of dipolar particles, where the polarization is induced by the external driving field. The neglected higher order terms describe the
effect of one polarized particle on the polarization of another, i.e., the local field effect. The same effect is at the heart of the Lorenz-Lorentz refractive index of a dielectric medium. We will later discuss in which parameter regime the local field effect becomes significant and present a systematic derivation of an effective two-body Hamiltonian.

6.3 Mean-field approximation

In the following we use the mean-field model established for a thermal atom cloud in Section 2.2.1, however we include the mean-field dipole-dipole potential besides the trap potential in three dimensions. The conservative dipole trap potential is

\[ V_{\text{trap}}(r) = \frac{\hbar \Omega^2}{\Delta_A} f^2(r). \]  

(6.14)

The mean-field dipole-dipole potential is

\[ V_{\text{dd}}^{(0)}(r) = -2\hbar^2 \frac{\Omega^2}{\Delta_A} f(r) \int d^3 \mathbf{r}_2 \ p(\mathbf{r}_2) \beta(\mathbf{r} - \mathbf{r}_2) f(\mathbf{r}_2), \]  

(6.15)

where the continuous position distribution \( p(\mathbf{r}) \) was introduced. This distribution is normalized to the number of atoms in the trap \( N \). The convolution integral can be evaluated as a product in Fourier space \([154, 157]\).

Assuming that the cloud of atoms is described by a canonical ensemble at an equilibrium temperature \( T \), the canonical distribution provides a self-consistent equation for the spatial distribution of the atoms:

\[ p(r) = \frac{1}{\mathcal{Z}} \exp \left[ -\frac{V(r, p(r))}{k_B T} \right], \]  

(6.16)

where the partition function \( \mathcal{Z} \) ensures that the integral of \( p(x) \) gives the number \( N \) of atoms. This self-consistent equation for the atom distribution is the basic equation of our model, which can be solved only numerically.

The MF model can be expressed in terms of dimensionless parameters, which amounts to the identification of the relevant quantities describing the equilibrium of a trapped cloud of atoms. The dipole trap depth (see Eq. (6.14)) is set by the intensity and the detuning, however, in the self-consistent equation (6.16) it is compared to the temperature. None of the above quantities appears separately, thus it is appropriate to introduce the scaled intensity

\[ I = \frac{\hbar \Omega^2}{|\Delta_A| k_B T}. \]  

(6.17)
The depth of the MF dipole-dipole potential relative to the trap depth is determined by the product of the small parameter $\gamma/\Delta_A$ and the atom number $N$ through the atomic density $p(r)$ in Eq. (6.15). The appropriate parameter is then the scaled atom number
\[
\mathcal{N} = \frac{N\gamma}{|\Delta_A|}.
\]
(6.18)

With these two dimensionless parameters, $I$ and $\mathcal{N}$, the effect of all the relevant physical quantities can be described.

### 6.4 Stability analysis

We determine the solution of Eq. (6.16) by the iterative method discussed in Sec. 2.2.1. Initially we take the canonical distribution of a noninteracting gas in the dipole trap. The dipole-dipole interaction term given by the convolution integral in Eq. (6.15) is calculated then from this distribution. It is suitable to go into Fourier-space where the convolution is a simple product. The Fourier transform of the term $\beta(r)$ is known, cf. Eqs. (6.9) and (6.11), while the term $p(r)f(r)$ is transformed by numerical Fast Fourier Transform (FFT). Due to the finite support of the distribution $\hat{p}(k)$ and the mode function $\hat{f}(k)$, the singularity of $\beta(x)$, which appears as a non-decaying Fourier transform in momentum space, is automatically regularized. On transforming the product back to real space by FFT we get the dipole-dipole term. Adding it to the dipole trap term of Eq. (6.14) yields the total mean field potential which furnishes a new atomic distribution via the canonical form in Eq. (6.16). The resulting $p(x)$ can be used as the starting distribution in the next step of the iteration. Continuing the steps of iteration until convergence, one obtains the self-consistent solution of Eq. (6.16).

The iteration does not necessarily converge; instability can be induced by large enough atom number or intensity. The iteration method suggests that the instability occurs as a collapse of the atomic cloud due to self-contraction in the center of the trap. However, in the lack of a precise modeling of the collisional processes, the collapse itself cannot be accounted for by our approach. We must limit ourselves to determining the range of convergence.

The mean field dipole-dipole energy Eq. (6.15) depends on the shape of the atomic cloud. It has a cylindrical symmetry and the laser-induced polarization is radial, the optical field being transverse. For this polarization, it is the "pancake-shaped" trap where the dipole-dipole contribution to the MF potential is negative, deepening the trap depth in the center, so that the collapse of the cloud can be expected. The MF potential vanishes
Figure 6.1: The boundary of the stability range of the atomic cloud is shown in logarithmic phase diagram of the scaled intensity $I$ and the scaled atom number $\mathcal{N}$. The field polarization is circular in the $\hat{x} - \hat{y}$ plane, and the waist is $w/\lambda = 1.33$ (circle), 2.66 (triangle), 5.33 (diamond), and 10.66 (pentagon). Straight lines represent a fit on the numerical data. As shown with empty circles, below $I = 10$ the phase boundary deviates from the corresponding fitted line ($w/\lambda = 1.33$), which indicates the effect of untrapped atoms.

in the center for a spherical atom distribution (the refinement of this statement can be found in [163]). For a cigar-shaped cloud the MF dipole-dipole energy would be positive, repelling atoms from the center, and thus the instability we discuss in the following could not occur. Note that in usual considerations of dipolar quantum gases, the static dipole moment is taken, oppositely, in the axial direction and then the pancake-shaped cloud is stable against dipole-dipole attraction [153].

In Fig. 6.1 the stability range of the iterations is presented for circular polarization in the $\hat{x} - \hat{y}$ plane, and for beam waists $w = 1.33, 2.66, 5.33, 10.66$ in units of $\lambda$. On the two-dimensional plot for the scaled atom number and scaled intensity variables (“phase diagram”), border points of the stability region are shown and the convergent iterative solution of Eq. (6.16) exists in the region below the points. The border points can be well fitted by a power law dependence of the critical scaled intensity on the scaled atom number, $I \propto \mathcal{N}^{-c}$. The fit is represented by lines, the exponent is $c = 0.40(\pm 0.01)$. Shown only for the $w/\lambda = 1.33$ data with empty circles, the boundary bends away from the fitted straight line at the right-most end. This happens below a certain scaled intensity ($I < 10$), when a significant portion of untrapped atoms appear.

It is not shown in the figure, however, we obtained the same results for linear polar-
Figure 6.2: Left scale: Maximum density of the cloud, \( p(0) \) in units of \( 1/\lambda^3 \times \Delta_A/\gamma \), plotted against the scaled intensity \( I \) for \( w/\lambda = 1.33 \) (circle), 2.66 (triangle), 5.33 (diamond). The straight line is a fit on the \( w/\lambda = 5.33 \) data. The scaled atom number \( \mathcal{N} \) is set such that the system remains slightly below the critical point. Right scale: stars with a constant fit represent the MF dipole-dipole potential \( V_{dd}/k_B T \) calculated close to the boundary of the range of stability. The beam waist is \( w/\lambda = 5.33 \).

We also checked that the addition of an arbitrary constant to the Fourier transform \( \tilde{\beta}(k) \) does not appreciably shift the phase boundary. This justifies the neglect of any type of Dirac-\( \delta \) potential in the Hamiltonian, e.g., the contact potential [162] or \( s \)-wave scattering. Finally, the mutual effect of clouds in neighboring trapping sites of the optical lattice potential created by the field in Eq. (6.1) proved to be negligible with respect to the phase diagram: the instability arises from the short-range part \( (1/r^3) \) of the dipole-dipole coupling and is determined by the cloud at a single trapping site.

The dipole-dipole coupling enhances the trap depth in the center and increases the atom density there. The resulting self-contraction of the cloud is counteracted by the random motion of the atoms. We expect that instability occurs when the energy shift due to the dipole-dipole coupling exceeds the thermal energy of the atoms. The numerical approach has allowed us to confirm this expectation. In Fig. 6.2 the ratio of the dipole-dipole interaction potential and the thermal energy is plotted (with stars) on a logarithmic scale at the edge of the stable region (where still stable solution exists), and one finds \( V_{dd} \approx k_B T \) closely constant.

Accepting the instability condition \( V_{dd} \approx k_B T \), the critical exponent \( c = 0.4 \) can be obtained by simple arguments. It follows from Eq. (6.15) that \( V_{dd}^{(0)}(0)/k_B T \) is proportional
Figure 6.3: (Color online) The ratio of the MF dipole potential and the total potential at the origin as a function of the scaled intensity $I$ for $w/\lambda = 5.33$, and at fixed values of $N = 1, 2, 4 \times 10^{-5}$.

to $\mathcal{I}N$ times the convolution integral. Using the dominant term of the potential for the distribution, i.e., the trap potential in harmonic approximation, the resulting Gaussian distribution has a normalization factor proportional to $\mathcal{I}^{3/2}$. The remaining part is the convolution involving the function $\beta$ which is singular at the origin. Thus the main contribution must come from this small domain, the cloud size is irrelevant and the integral must be determined, at least to leading order, by the aspect ratio of the trapped cloud. Altogether $V_{dd}^{(0)}(0)/k_B T \propto \mathcal{I}^{5/2}N$ from which the scaling $\mathcal{I} \propto N^{-0.4}$ follows.

For consistency, let us check the validity of the effective Hamiltonian given in Eq. (6.13) which keeps only the leading order term of the dipole-dipole interaction. Figure 6.3 depicts the ratio of the MF dipole-dipole potential to the trap potential at the center of the cloud, which is the same ratio as that of the higher order terms of the polarization to the leading order one [cf. Eq. (6.12)]. This ratio grows as a function of the scaled intensity until reaching the critical point which is clearly manifested in this semi-logarithmic plot. The main thing to observe is that the criticality is reached at fairly low ratio of the dipole-dipole potential to the trapping one, at a value well below 0.1. Therefore, in the considered parameter regime, the leading order description is enough to find the boundary of the stability domain.
6.5 Possibility of Bose-Einstein condensation

The peak density is a key quantity with respect to reaching quantum degeneracy, which happens roughly at the density \( p(0) \lambda_{\text{deBroglie}}^3 \approx \zeta(3/2) = 2.612 \) [106], or, expressed in another way,

\[
p(0) \lambda^3 \approx 41 \left( \frac{T}{T_{\text{rec}}} \right)^{3/2},
\]

where \( T_{\text{rec}} = (\hbar^2 k^2/m) / k_B \) is the recoil temperature. This condition depends, separately, on the temperature which has been, so far, embedded in the scaled intensity. Therefore, depending on the working point, i.e. the actual value of the temperature and the trap depth, the order of reaching quantum degeneracy or reaching the dipole-dipole instability can be chosen.

Obviously, both increasing the trap depth (at fixed temperature) and increasing the absolute atom number (at fixed detuning) lead to an increase of the density at the trap center. However, the critical behavior can be induced at different peak densities depending on how it is obtained: whether by increasing \( I \) or \( N \). We present in Fig. 6.2 the calculated peak densities along the phase boundary, i.e., for clouds which are infinitesimally close to the boundary of the stable phase. The numerical values obtained for various waists overlap, and can be well fitted by a power law function \( 1/I \). Thus the dipole-dipole instability appears at densities

\[
p(0) \lambda^3 \approx \frac{\lambda_A}{\gamma} I, \quad (6.20)
\]

We recall that the dimensionless detuning \( \lambda_A/\gamma \) describes the ratio of the dipole trap potential depth and the spontaneous photon scattering rate. Thus if the right-hand-side of the inequality (6.20) is smaller than that of (6.19), the dipole-dipole instability prevents that the limit of quantum degeneracy could be reached. For example, with atoms at about 100 \( \mu K \), 3 orders of magnitude above the (typical) recoil temperature, and for \( I = 10 \) (trap depth about mK), one needs a detuning \( \lambda_A > 10^5 \gamma \) so that the Bose-Einstein condensation point falls into the stability range of the dipole-dipole interaction. On increasing the scaled intensity \( I \), the threshold density \( p(0) \) for the dipole-dipole instability decreases (see Fig. 6.2 and Eq. (6.20)), which amounts to a more demanding condition on the atom number or on the temperature needed to achieve condensation.

\[
\frac{\lambda_A}{\gamma} = \frac{\lambda_A}{\gamma} I
\]

\[
\frac{\lambda_A}{\gamma} I = \frac{\lambda_A}{\gamma} I
\]
6.6 Summary

I set up a simple but versatile model to study the stability of far-off-resonance trapping against the dipole-dipole interaction. The model can be adapted to various geometries, atomic species and polarizations. I found that the radiative atom-atom interaction in the laser polarized gas can indeed produce an instability of a pancake-shaped atomic cloud. When the dipole-dipole energy shift reaches the temperature, the unbalanced attraction in the trap center yields a collapse of the cloud. The condition for the instability in terms of the atom density and the temperature is obtained numerically in the form of phase diagrams.

The density necessary for large enough dipole-dipole shift is quite large, however, the temperature is not needed to be very low so that the instability be observable. Provided the optical dipole trap is deep enough, the stability can be lost at moderate phase-space densities, well above the condensation threshold. On the other hand, it is also possible to find a working point, very large detuning, low temperature and not too large trap depth, where the dipole-dipole coupling itself does not prevent the gas from forming a quantum degenerate state.
Chapter 7

Summary

Many-body physics with cold and ultracold atomic gases has been an expanding field of research over the past decades. These systems are especially appealing because they constitute good quantum simulators, meaning that fundamental problems can be addressed in well-controlled experiments.

In this Thesis, I focused on the collective effects that stemmed from the atom–atom interactions mediated by the radiation field. I concentrated solely on the dispersive regime, where the atoms were treated as polarizable particles with real refractive index. In the major part of the Thesis, I considered the case where the atoms coupled to a few cavity field modes. The resulting infinite-range atom–atom interaction produced a phase transition between a homogeneous spatial distribution and a regular periodic pattern. I studied this self-organization effect by a mean-field approach both for cold and ultracold atomic samples, i.e. for a thermal cloud of atoms and for a zero-temperature Bose-Einstein condensate.

The other focus of this work was on the quantum fluctuations of a BEC inside an optical resonator. Photon field of the cavity couples to the excitations of the condensate, hence polariton modes appear in the collective excitation spectrum of the system. They inherit the properties of the cavity mode, therefore they are lossy and they are driven by the quantum fluctuations accompanying the photon loss. I investigated the steady-state properties of these polariton modes as well as the transient quantum dynamics of the one which dominantly couples to the cavity field. The steady-state atomic population in the excitations accounts for the condensate depletion. Whereas, the BEC excitation mode coupling dominantly to the cavity field realizes the opto-mechanical coupling, however, in a different regime that is studied with oscillating mirrors coupled to the field of high-finesse cavities.
Finally, I dealt with the induced dipole-dipole interaction in the context of the far-off-resonance optical dipole trapping scheme. This long-range atom–atom interaction is mediated by the free space radiation modes. The dipole-dipole energy shift yields an attractive mean-field contribution to the trapping potential, hence it can lead to the collapse of the atom cloud when the maximum atom density in the trap reaches a critical value.

The main results of this Ph.D. Thesis are summarized in the following points:

I Using a mean-field approach, I studied the spatial self-organization of a cold gas of linearly polarized particles transversely pumped by an off-resonant laser and interacting with the counterpropagating radiation modes of a high-$Q$ optical ring resonator. In the thermodynamic limit, the canonical distribution together with the optical dipole potential exerted on the atoms by the cavity field provides a self-consistent equation for the density of the gas, that I solved by an iterative numerical method. I found three stable thermodynamic phases: i) a uniform distribution, ii) a self-organized Bragg-lattice and iii) a lattice with defects. I mapped these phases on a phase diagram as a function of the pump strength and the particle density [91].

II In terms of the Gross-Pitaevskii mean-field theory, I described the self-organization of a Bose-Einstein condensate laser-driven from the transverse direction and dispersively interacting with the field of a high-finesse linear optical cavity. Above a critical pump intensity, the homogeneous condensate evolves into a stable pattern, whose periodicity is given by the cavity wavelength. The analytic expression for the transition point reveals that below threshold the homogeneous phase is stabilized mainly by the atom–atom collisions besides the small kinetic energy of the gas [92].

III Considering small fluctuations around the mean-field solution, I calculated the collective excitation spectrum of the BEC–cavity system in the transverse pumping geometry. The critical point of self-organization is clearly manifested in the spectrum by the degeneracy of one excitation mode with the ground state of the system. Below threshold, I obtained the spectrum analytically. Above threshold, the spectrum qualitatively depends on the density of the atoms, because in the strong coupling regime, where classically defect sites appear in the optical potential, new type of BEC excitations can take place [92].

IV Quantum fluctuations of the resonator field drive the excitation modes of the compound BEC–cavity system, which results in a finite number of atoms outside the
macroscopically occupied condensate state. For cavity pumping, I determined this excess noise depletion in the steady state by solving the Heisenberg-Langevin equations for the quasinormal mode excitations. In the weak coupling limit, I obtained both analytical and numerical results. I found that the steady-state depletion depends mostly on the cavity detuning and photon loss rate setting the noise level in the system. The depletion is independent of the total number of atoms, and it does not significantly depend on the strength of the atom-field interaction and on the photon number [93].

V I derived a quantum master equation for a single mode excitation of a Bose-Einstein condensate by an optical cavity mode. The presented model originates from the opto-mechanical coupling between the atom and radiation field modes, however the cavity field is eliminated from the system. The resulting equation for the single BEC excitation mode accounts for the dissipative part of the dynamics including friction and diffusion effects. By the numerical simulation of the master equation, I found that the measurement-induced back-action noise impedes the observation of quantum tunneling in the classically bistable regime. Nevertheless, coherent matter wave oscillations are possible, where diffusion leads to a non-exponential dephasing effect, whose magnitude decreases with the increase of the oscillation amplitude [94].

VI In a mean-field approach, I calculated the effect of the dipole-dipole interaction on the far-off-resonance optical dipole trapping of cold atoms. I found that the mean-field interaction energy is negative for a pancake-shaped cloud, therefore it deepens the center of the trap potential. Above a critical peak density, the thermal motion cannot stabilize the gas against self-contraction and an instability occurs, which manifests itself in the collapse of the cloud. The boundary of the stable equilibrium region expressed in terms of the ratio of the trap depth to the temperature shows a power law dependence on the atom number with exponent $-0.4$. I determined the maximum achievable peak density in a dipole trap as a function of the system parameters and compared it to the limit of quantum degeneracy [96].
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Bibliography


List of publications

Publications in the subject of this Thesis


Further publications out of the scope of this Thesis
