

Classical and Quantum Parametric Excitations of Bose-Einstein Condensates

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December 1, 2016

Abstract

In this thesis, we study the parametric excitations of a homogeneous Bose-Einstein condensate (BEC) at finite temperature obtained from modulating the interaction strength.

In Bogoliubov theory, a result connecting the real part of the diagonal Bogoliubov coefficient and instability, i.e. exponential growth of excitations, is obtained for general periodic modulations. Consequently, an analytic solution for an arbitrary square wave modulation is derived that can be studied to understand similar drivings like the sinusoidal case. This adds to previous works studying only the case for small driving amplitudes.

In the recent experimental and theoretical literature well-established nonclassicality criteria from the field of quantum optics have been directly applied to the case of excitations in matter-waves like those studied here. Among these are violations of Cauchy-Schwarz inequalities, Glauber-Sudarshan P-nonclassicality, sub-Poissonian number-difference squeezing (also known as the two-mode variance) and the criterion of nonseparability. We review the strong connection of these criteria and their meaning in quantum optics, and point out differences in the interpretation between light and matter waves.

By proposing a classical theory of a thermal BEC that gives the same predictions as the quantum theory in the high temperature limit, and using it as a reference, we can isolate real quantum effects like spontaneous emission caused by quantum noise.

We conclude that to date in experiments relevant for this scenario nonclassical effects have not conclusively been observed and conjecture that additional, noncommuting, observables have to be measured to this end. Moreover this has important implications for proposed analog gravity models where the observation of nonclassical effects is a major goal.

In the second part of the thesis, we present simulational methods with focus on the Truncated Wigner Approximation (TWA). We take a path integral approach inspired by [Polkovnikov, 2010] and derive a set of classical equations from the semi-classical limit that is more general than TWA. We add some proofs to the literature and identify problems in this approach.

We also present a highly optimized software package as an extension of previous work [Jain, 2007]. It can carry out the relevant simulations and we use it to confirm the theoretical predictions of the first part.

Acknowledgements

I would like to first thank my supervisors Silke Weinfurter and Peter Krüger: Silke for showing me the value of creativity for science, for sharing fascination and sparking motivation, and various small and large pieces of help along the way of becoming sort of a scientist myself; Peter for always openly sharing with me deep physical insights as well as a marvellously liberal view of the world, and further for professional management of the most complicated issues in a most likely optimal way.

Both have continuously impressed me with their physical intuition and asking the right questions, which often lead me to a deeper understanding and which definitely has opened up my approach to problem solving.

For friendship I would in particular like to thank Giannis Kogias and Alban Levity. Their encouragement was crucial for the completion of this thesis. This work also profited directly from many discussions about quantum physics with Giannis.

Of course, there were many more people in and outside of Nottingham and Trieste from which I have learned or who have otherwise enriched my life, and who are all somehow connected in my mind to this thesis due to the blurred boundaries between private and professional life, and I am thanking all of them.

Finally, I thank my parents Pia and Klaus Finke for their unconditional love, for letting me pursue my dreams, helping where they can without asking for anything in return but my happiness.

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Part I.

Introduction: The Notion of Nonclassicality

Bose-Einstein condensation (BEC) is a macroscopic quantum phenomenon where a large fraction of the bosons occupy the same lowest energy quantum state, and thus form a coherent matter wave. Many properties of the condensate can be captured by a Schrödinger-type equation for a complex field with a nonlinear potential referred to as the Gross-Pitaevskii equation (GPE) [Davis et al., 1995, Castin, 2001, Polkovnikov, 2010]. To cite one example, the GPE correctly predicts discrete values for the circulation of the velocity field in a BEC [Fetter, 2009]. Nevertheless, within this description the evolution of the condensate can be considered a classical process [Johnson et al., 2014]. On the other hand it is possible to excite small fluctuations of the condensate, for example by means of rapid changes in the condensate parameters [Bauer et al., 2009, S. Inouye and Ketterle, 1998, Jaskula et al., 2012, Steinhauer, 2014, Steinhauer, 2016, Steffens et al., 2014], which may activate their nonclassical behaviour. An ongoing line of research is to investigate experimentally the manipulation and detection of fluctuations in BECs, e.g. exploring their quantum nature [Krachmalnicoff et al., 2010, Jaskula et al., 2010, Kheruntsyan et al., 2012] and correlations [Schweigler et al., 2015, Steffens et al., 2014]. This is partially motivated by various analogue gravity studies [Unruh, 1981, Barceló et al., 2011, Schützhold and Unruh, 2007, Faccio et al., 2013], where BECs are utilized as quantum simulators [Johnson et al., 2014] of quantum field theories in curved spacetime (QFTCS). In QFTCS one is interested in how quantum fields propagate on a classical curved spacetime geometry acting as a non-trivial background configuration. Within analogue gravity studies the ultimate goal is to mimic and capture genuine quantum effects predicted from QFTCS. The field of experimental analogue gravity in BECs started only a few years ago, and with recent advances, e.g. mimicking black hole evaporation [Steinhauer, 2014, Steinhauer, 2016, Lahav et al., 2010, Coutant and Parentani, 2010, Finazzi and Parentani, 2010] and cosmological particle production in our universe [Jaskula et al., 2010, Hung et al., 2013, Jain et al., 2007, Carusotto et al., 2010, Busch et al., 2014], the debate on the nonclassicality of the observed effects is as timely as ever. Hence, it is essential to find suitable observables that can distinguish between classical and nonclassical features of excitations in the condensate.

A well-defined notion of *nonclassicality* or *quantumness* for any physical system, governed by the laws of nature, which ultimately are laws of quantum physics, can only come about by

comparing to a *classical reference* – a certain theoretical framework making predictions for experiments which is known *not* to fully capture all of the physics. Experimental outcomes that are incompatible with this reference are falsifying it; they may be said to *be nonclassical*.

For some, but not all, fields of physics, established choices exist for the classical reference. This is usually due to the historic development of the particular field. For example, in optics, the semiclassical theory of the classical (but stochastic) electromagnetic field interacting with atoms (modelled by quantum mechanics) is a commonly employed classical reference when talking about light. From this perspective, observed properties of states with small photon number can be nonclassical.

Once a well-defined notion of nonclassicality is established, physically sensible *nonclassicality criteria for quantum states* may be defined. The goal is to assess the utility of a quantum state for the falsification of the classical reference. Thus, for the present example of quantum optics, states with low photon number should be among the states singled out by such a criterion. Far more generally, in the recent quantum information literature, mathematical properties of certain quantum states are often given names suggesting nonclassical behavior of any system described by such a state. Examples of such properties are nonlocality [Brunner et al., 2014], quantum steering [Wiseman et al., 2007, Skrzypczyk et al., 2014], nonseparability (entanglement) [Werner, 1989, Horodecki et al., 2009], quantum discord [Ollivier and Zurek, 2001] and quantum coherence [Adesso et al., 2016]. The viewpoint we are taking here – asking for the measurable effects that cannot be accounted for by some classical reference – is strongly related to the so-called *operational* understanding of such properties of states. This is subject to current research, motivated in part by seeking applications for quantum computation and quantum cryptography.

A concrete and prominent example for a nonclassicality criterion from optics in the setting of (joint) photon counting experiments is the non-existence of a positive Glauber-Sudarshan or P-distribution [Titulaer and Glauber, 1965, Sudarshan, 1963] (a mathematical statement that can be checked for any quantum state), and various theoretical and experimental criteria derived from it [Kiesel et al., 2008]. As we are going to see below, these criteria do possess an operational foundation based on the effects of the destructive measurement of photons.

These effects are not contained in the semi-classical theory. For example, the joint click rate for two detectors is zero in a single photon state, but nonzero for each individual detector, which cannot be understood in a wave theory of light.

It is necessary to distinguish between two subtly different types of experiments regarding nonclassicality. On the one hand, there are experiments (of type A, say) that directly, by utilizing a nonclassical state, falsify the classical reference (e.g. photoelectric effect, photon anti-bunching). On the other hand, there are experiments (of type B) that indirectly probe some properties of the state to establish its nonclassicality. By this we mean that it is logically possible that an experiment of type B does not witness any nonclassical behavior, but is still sufficiently tomographic to enable the experimentator to understand that the state is indeed a *nonclassical state* according to the notions we have introduced, i.e. a state which would *show nonclassical behavior* – by falsifying the classical reference – directly only in *another* experiment of type A.

These different types of experiments are totally different in their interpretation and the associated required theoretical effort. Note that for the falsification of the classical reference with experiments of type A, all that is needed is the evaluation of the experiment within that reference. Bounds on the data that are predicted within the classical reference may be violated by the measured data. An understanding of a more realistic model is not strictly needed to falsify a given model. On the other hand, in the case of experiments of type B, a detailed quantum theoretical understanding of the experiment, including perhaps even an understanding of the environment-induced decoherence, are crucial to enable sufficiently accurate state tomography for a correct interpretation of the results. As a simple example, measuring the outcome of each of two possible results of a spin-1/2 system with equal probability does not allow us to conclude that a previously prepared equal-weighted superposition still is in a coherent pure state, since it could have been decohered to a mixed state. Trusting the coherence is only possible after many more experiments, involving those of type A, have been carried out to verify it directly.

The physically sensible application of nonclassicality criteria from quantum optics to the field of matter wave optics is conceptually not straightforward, even if in full analogy to

optics we choose as a classical reference a wave theory as well, namely, naturally, the semiclassical GPE description of the BEC. This is, first of all, because of the restricted set of measurements commonly available, causing difficulty in finding experiments of type A. Second, generally present interactions would in principle require a complicated analysis for predicting the experimental results in either framework (for experiments of type B). (Note also that the linearity of standard quantum optics is enabling us to obtain accurate theoretical predictions with relative ease for many experiments in the optical setting.) In particular, it was shown in [Finke et al., 2016], that simple correlation measurements of atom numbers in two different momentum modes, which were two-mode squeezed, are not an experiment of type A, but at most of type B for assessing the nonclassicality of the state for any values of initial temperature and squeezing. This is so despite the quantum state being nonseparable with respect to the two modes for sufficiently strong squeezing and number correlations within a restricted analysis in second quantized Bogoliubov theory which, of course, neglects the interactions and decoherence. Only if this analysis is experimentally proven to be correct can such a number correlation experiment be taken as an experiment of type B. At present, as pointed out in [Finke et al., 2016], *no* experiment of type A is known, which could clearly distinguish between the mean-field GPE description of the excitations and the quantized Bogoliubov excitations for motional modes (as opposed to correlations between states for an internal degree of freedom, for which Bell inequality violations have recently been observed [Schmied et al., 2016]).

This lack of suitable experiments for nonclassicality might be an explanation for why it is that simulational methods based on classical fields so far describe most experiments well. However, with the Truncated Wigner method (as well as related methods based on phase space representations of quantum mechanics), there exists a method that within some limits should produce more than classical results. The study of true quantum effects can then be taken as a benchmark for such methods.

Part II.

Nonclassicality in Parametrically Excited Matter-Waves

1. Parametric Resonance

1.1. Set-up

We focus on the case of the finite-temperature homogeneous BEC undergoing parametric excitations due to an arbitrary periodic variation of the scattering length. This has the advantage of allowing to strongly drive selected modes of the system to amplify their occupation number, and from an experimental perspective this can be implemented straightforwardly, see for example [Bauer et al., 2009, S. Inouye and Ketterle, 1998, Hung et al., 2013]. We analyze the stability and growth rates for modes under periodic driving. First, we consider the quantum case. The system is described assuming quadratic Bogoliubov theory, which neglects phonon interactions, so that the non-equilibrium dynamics can be solved exactly. Within this approximation initially Gaussian quantum states remain Gaussian. As a classical reference we employ a quadratic semiclassical approach based on the GPE with an initial thermal mode population which also preserves Gaussianity. The equations of motion for the classical case will turn out to have the same form as in the quantum case, and the stability analysis for the latter given next will also apply for the classical case.

1.2. Quantum Theory

We consider an interacting Bose gas in a box of volume $V = L^d$ with time-dependent interaction strength. The second quantized Hamiltonian is given by

$$\hat{H}(t) = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \frac{U(t)}{2V} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \hat{a}_{\mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\mathbf{k}} \hat{a}_{\mathbf{k}'}, \quad (1.1)$$

where $\hat{a}_{\mathbf{k}}$ annihilates a single particle eigenstate of the (translationally invariant) momentum operator and $\mathbf{k} \in 2\pi\mathbb{N}^d/L$. To simplify the discussion, we set $d = 3$ in this part of the thesis and assume the box to be large enough to approximate its single particle ground state by $\hat{a}_{\mathbf{0}}^\dagger |0\rangle$. For atoms of mass m and s-wave scattering valid in the ultracold regime, the effective interaction is $U(t) = 4\pi\hbar^2 a_s(t)/m$. In experiments, the time-dependence of the scattering length $a_s(t)$ can be achieved by use of an appropriate Feshbach resonance [S. Inouye and Ketterle, 1998, Roberts et al., 2001]. We assume all changes to be slow enough not to excite the bound state of the resonance [Corson and Bohn, 2015].

1.2.1. Quasiparticles

Our formulation is based on standard Bogoliubov theory valid for a weakly interacting Bose gas [Dalfovo et al., 1999]. The Hamiltonian can be diagonalized by retaining only interaction terms to quadratic order in the total number of particles N after the Bogoliubov approximation

$$\hat{a}_{\mathbf{0}} = \hat{a}_{\mathbf{0}}^\dagger = \sqrt{N - \Delta}. \quad (1.2)$$

With the critical assumption of a small depletion of the condensate, i.e. $\Delta = \sum_{\mathbf{k} \neq 0} \langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \rangle \ll N$, the Hamiltonian becomes a quadratic expression in the mode operators. Only modes with opposite momenta are coupled in a homogeneous condensate and we henceforth use the abbreviated notation $\hat{a} \equiv \hat{a}_{\mathbf{k}}$ and $\hat{b} \equiv \hat{a}_{-\mathbf{k}}$. A two-mode squeezing represented by the transformation

$$\begin{aligned} a &= u_k(t) \hat{A} + v_k(t) \hat{B}^\dagger; \\ b^\dagger &= u_k(t) \hat{B}^\dagger + v_k(t) \hat{A}, \end{aligned} \quad (1.3)$$

can be used to diagonalise the Hamiltonian, where the coefficients only depend on $k \equiv |\mathbf{k}|$. The coefficients may further be chosen as real numbers satisfying $u_k^2 - v_k^2 = 1$. Then the transformation is a Bogoliubov transformation, i.e. leaves the bosonic commutation relation unchanged, $[\hat{A}, \hat{A}^\dagger] = 1 = [\hat{B}, \hat{B}^\dagger]$, and $[\hat{A}, \hat{B}] = 0$. Neglecting the ground state energy the Hamiltonian $\hat{H}(t) = \sum_{\mathbf{k}} \hbar\omega_k(t) \hat{A}^\dagger(t) \hat{A}(t)$ counts the elementary excitations of the system,

the so-called quasiparticles, with

$$u_k(t), v_k(t) = \frac{1}{2} \left(\frac{e_k^{\text{kin}}}{e_k(t)} \right)^{1/2} \pm \frac{1}{2} \left(\frac{e_k(t)}{e_k^{\text{kin}}} \right)^{1/2}, \quad (1.4)$$

with density $n = N/V$, kinetic energy $e_k^{\text{kin}} = \hbar^2 k^2 / 2m$ and

$$e_k(t) = \hbar \omega_k(t) = \sqrt{e_k^{\text{kin}} (e_k^{\text{kin}} + 2U(t)n)}, \quad (1.5)$$

the well-known Bogoliubov dispersion relation. Assuming the equilibrated isolated system can be treated in the canonical ensemble with respect to the particles (or grand canonical with respect to the quasiparticles with vanishing chemical potential as their number is not conserved), with the density operator $\hat{\rho}_{th} \propto \exp(-\hat{H}/k_B T)$,

$$\langle \hat{A}^\dagger \hat{A} \rangle_{th} = \frac{1}{\exp(\hbar \omega_k / k_B T) - 1} =: n_k^{th}, \quad (1.6)$$

and the anomalous quasiparticle average $\langle \hat{A} \hat{B} \rangle_{th} = 0$. (Note that although we are neglecting the interactions between the quasi-particles, we do assume their presence at longer time-scales, allowing the condensate to thermalise in the first place.) For continuous time dependence of $U(t)$ the Heisenberg equations for the operators are, with $S(t) = (\hat{A}(t), \hat{B}^\dagger(t))^T$, given by $dS/dt = M(t)S$ where

$$M(t) := \begin{pmatrix} -i\omega_k & \frac{d \log \sqrt{\omega_k}}{dt} \\ \frac{d \log \sqrt{\omega_k}}{dt} & i\omega_k \end{pmatrix}. \quad (1.7)$$

The derivation of this compact form of the equations is lengthy but straightforward with the identities $\dot{u}_k v_k - \dot{v}_k u_k = -\dot{v}_k / u_k = -\dot{v}_k / u_k = \dot{\omega}_k / 2\omega_k$ (using the time derivative of the equation $u_k^2 = 1 + v_k^2$).

This implies that it is possible in general to describe the time evolution by a further linear transformation of the form

$$\begin{aligned} \hat{A}(t^{\text{out}}) &= \alpha_k^* \hat{A}(t^{\text{in}}) + \beta_k \hat{B}^\dagger(t^{\text{in}}); \\ \hat{B}^\dagger(t^{\text{out}}) &= \alpha_k \hat{B}^\dagger(t^{\text{in}}) + \beta_k^* \hat{A}(t^{\text{in}}). \end{aligned} \quad (1.8)$$

The complex coefficients α_k^* , β_k and α_k , β_k^* are the entries of the first and of the second row of the fundamental matrix $\varphi(t = t^{\text{out}})$ respectively, that is,

$$\begin{aligned} d\varphi(t)/dt &= M(t)\varphi(t) \\ \varphi(t^{\text{in}}) &= \mathbf{1}_{2 \times 2} \end{aligned} \quad (1.9)$$

and

$$\varphi(t^{\text{out}}) \equiv \begin{pmatrix} \alpha_k^* & \beta_k \\ \beta_k^* & \alpha_k \end{pmatrix}. \quad (1.10)$$

Using $\det(\varphi) = \exp(\text{tr}(\log(\varphi)))$ we have

$$\begin{aligned} d/dt(|\alpha_k|^2 - |\beta_k|^2) &= d/dt \det(\varphi) \\ &= \det(\varphi) \text{tr}(\varphi^{-1} M \varphi) \\ &= 0 \end{aligned} \quad (1.11)$$

since $\text{tr} M = 0$ for all t . Thus, at all times $|\alpha_k|^2 - |\beta_k|^2 = 1$ and (1.8) is a Bogoliubov transformation. We choose with no loss of generality $t^{\text{out}} = 0$ such that for $t > 0$ the interaction strength is kept constant, defining the *out*-region, in which the time evolution is a trivial phase oscillation. Note that the arbitrary time dependence of $U(t < 0)$ is now encoded in the complex Bogoliubov coefficients α_k and β_k subject to the normalisation constraint. The dependence of these coefficients on $U(t < 0)$ is implicit in our notation.

1.2.2. Instabilities

By a periodic modulation of the interaction strength, $|\beta_k|$ grows exponentially with the number of periods if k is in a region of instability. For example, for low amplitude sinusoidal modulations of the form $U(t) = U_0(1 + A \sin(\omega_D t))$ with $A \ll 1$ the first resonance occurs at $\omega_k = \omega_D/2$ [Staliunas et al., 2002].

More generally, the fundamental matrix propagating the solution from the beginning of the modulation to the end at $t = 0$ can be obtained by multiplying together the fundamental matrices belonging to the elements of any decomposition of this time interval into multiple shorter intervals. For N modulation periods of length T each, we can write $\varphi(0) = \phi^N$ where

$$\phi \equiv \begin{pmatrix} \alpha_T^* & \beta_T \\ \beta_T^* & \alpha_T \end{pmatrix} \quad (1.12)$$

is the solution of system (1.9) integrated for a single period. If this is implemented numerically, this speeds up the integration times at constant accuracy by at least a factor of N . Information

on the behavior of the total Bogoliubov coefficients can be read off directly from those of the single period. These results are obtained by diagonalizing a general ϕ to calculate ϕ^N . Furthermore, explicit analytic results may be obtained in the case of a square wave modulation, when ϕ itself is analytically known.

For the diagonalization of ϕ , we begin with the eigenvalues of ϕ ,

$$\lambda_{1/2} = \text{Re } \alpha_T \pm \sqrt{(\text{Re } \alpha_T)^2 - 1}, \quad (1.13)$$

which obey

$$\lambda_1 + \lambda_2 = \alpha_T + \alpha_T^* \quad (1.14)$$

$$\lambda_1 \lambda_2 = 1, \quad (1.15)$$

and do not depend on β_T . The overall Bogoliubov coefficients (the entries of $\varphi(0) = \phi^N$) can then be shown to read

$$\beta_k = \frac{\lambda_1^N - \lambda_2^N}{\lambda_1 - \lambda_2} \beta_T \quad (1.16)$$

$$\alpha_k = \frac{\lambda_1^N - \lambda_2^N}{\lambda_1 - \lambda_2} \alpha_T + \frac{\lambda_2^{N-1} - \lambda_1^{N-1}}{\lambda_1 - \lambda_2}. \quad (1.17)$$

Note that for $|\text{Re } \alpha_T| < 1$ the eigenvalues have a non-vanishing imaginary part and $\lambda_1 = \lambda_2^*$. Then equation (1.15) implies that they are phases on the unit circle in the complex plane. The total Bogoliubov coefficients oscillate with increasing N in this case. On the other hand, for $|\text{Re } \alpha_T| > 1$ exponential growth will take place, and this inequality is thus the condition for instability. Indeed, in this case we can define $\lambda \equiv \max(\lambda_1, -\lambda_2) = |\text{Re } \alpha_T| + \sqrt{(\text{Re } \alpha_T)^2 - 1} > 1$ and we find with equation (1.15), and defining $s \equiv \text{sign}(\text{Re } \alpha_T)$,

$$\beta_k = s^{N+1} \frac{\lambda^N - \lambda^{-N}}{\lambda - \lambda^{-1}} \beta_T \quad (1.18)$$

$$\approx \frac{s^{N+1} \lambda^N}{\lambda - \lambda^{-1}} \beta_T \quad (N \gg 1) \quad (1.19)$$

$$\alpha_k = \frac{s^{N+1}}{\lambda - \lambda^{-1}} \left((\lambda^N - \lambda^{-N}) \alpha_T - s(\lambda^{N-1} - \lambda^{-(N-1)}) \right) \quad (1.20)$$

$$\approx \frac{s^{N+1} \lambda^{N-1}}{\lambda - \lambda^{-1}} (\lambda \alpha_T - s) \quad (N \gg 1), \quad (1.21)$$

and we see that exponential growth occurs asymptotically as $\propto \lambda^N = e^{t/T \log \lambda}$.

In the limit $|\operatorname{Re} \alpha_T| \rightarrow 1+$, the factor $1/(\lambda - \lambda^{-1})$ is divergent, and one cannot use this asymptotic expression. However, one can show that $|\beta_k| = |\beta_T|((\lambda^N - \lambda^{-N})/(\lambda - \lambda^{-1})) \rightarrow |\beta_T|N$, that is, a regime of linear instead of exponential growth is approached for very small growth rates as expected.

Since λ is strictly increasing with $|\operatorname{Re} \alpha_T|$, the main resonance will (for sufficiently large N and if there is a unstable region) simply be given by the k that extremizes $|\operatorname{Re} \alpha_T|$.

It is also interesting to note that the phase of β_k is the same as the phase of β_T for all N , and the phase of α_k is approaching a constant for large N .

We have seen that all information about the growth rates and thus, for large N , the position in k -space of the resonance peaks, is contained in $\operatorname{Re} \alpha_T$ for a single step. The Bogoliubov coefficients can be obtained for each k separately from integrating (1.9), or alternatively from integrating the following two decoupled second order equations for two real auxiliary functions ρ and σ , which are obtained after suitable transformation from the two equations in (1.9) for the real part of α_T ,

$$\ddot{\rho} - \dot{U}f_k(t)\dot{\rho} + \left(\omega^2 + \frac{5}{4}(\dot{U}f_k(t))^2 - \frac{1}{2}\ddot{U}f_k(t) \right) \rho = 0 \quad (1.22)$$

$$\ddot{\sigma} - \dot{U}f_k(t)\dot{\sigma} + \left(\omega^2 - \frac{7}{4}(\dot{U}f_k(t))^2 + \frac{1}{2}\ddot{U}f_k(t) \right) \sigma = 0. \quad (1.23)$$

The integration is from $-T$ to 0, and $f_k(t) \equiv ne_k^{\text{kin}}\omega^{-2}$, $\omega = \omega(k, t)$, $U = U(t)$, $\rho(-T) = 1$, $\dot{\rho}(-T) = \dot{\omega}(-T)/(2\omega(-T))$, $\sigma(-T) = 1$, $\dot{\sigma}(-T) = -\dot{\omega}(-T)/(2\omega(-T))$. We then find $\operatorname{Re} \alpha_T = \rho(0) + \sigma(0)$.

In the phononic regime $e_k^{\text{kin}} \ll Un$, the substitution $\tilde{\rho} = \rho U^{-1/4}$, $\tilde{\sigma} = \sigma U^{1/4}$ gives the equations

$$\ddot{\tilde{\rho}} + k^2 e^{g(t)} \tilde{\rho} = 0 \quad (1.24)$$

$$\ddot{\tilde{\sigma}} - \dot{g}(t)\dot{\tilde{\sigma}} + k^2 e^{g(t)} \tilde{\sigma} = 0 \quad (1.25)$$

in standard form, again to be integrated from $-T$ to 0, and where $g(t) \equiv \log(U(t))$, $\tilde{\rho}(-T) = U^{-1/4}(-T)$, $\dot{\tilde{\rho}}(-T) = 0$, $\tilde{\sigma}(-T) = U^{1/4}(-T)$, $\dot{\tilde{\sigma}}(-T) = 0$ and $\operatorname{Re} \alpha_T = \tilde{\rho}(0)U^{1/4}(0) + \tilde{\sigma}(0)U^{-1/4}(0)$.

1.2.3. Analytic Results for Periodic Driving

Square-wave Modulation

First we are considering the case of rectangular periodic variation of the interaction strength explicitly, that is $2N$ quenches with the interaction strength jumping between U_1 and U_2 with a separation in time of $\tau \equiv T/2$. We are left with the task to calculate α_T and β_T for a period consisting of two quenches and two free phase evolutions.

For a single quench at $t = t_q$ from U^{in} to U^{out} , consider the particle operators on the left hand side of equation (1.3). Imposing their continuity at $t = t_q$ (the Hamiltonian is bounded at all times and thus, according to the Heisenberg equations of motion for the *not* explicitly time-dependent particle operators, their rate of change is bounded, so that the total change is proportional to the evolution time to first order, which is zero for the quench), we find relations between the *in* and *out* quasiparticle operators which can be compared with equation (1.8) to calculate readily, employing equations (1.4),

$$\mathfrak{A}_k, \mathfrak{B}_k = \frac{1}{2} \left(\frac{\omega_k^{\text{out}}}{\omega_k^{\text{in}}} \right)^{1/2} \pm \frac{1}{2} \left(\frac{\omega_k^{\text{in}}}{\omega_k^{\text{out}}} \right)^{1/2}, \quad (1.26)$$

as the (real) Bogoliubov coefficients transforming the quasiparticle operators directly before the quench to those directly afterwards. We define the corresponding matrix (which can also be derived as the fundamental matrix of a piecewise linear change of duration δt in the limit $\delta t \rightarrow 0$):

$$\Gamma[\omega^{\text{in}} \rightarrow \omega^{\text{out}}] := \begin{pmatrix} \mathfrak{A}_k & \mathfrak{B}_k \\ \mathfrak{B}_k & \mathfrak{A}_k \end{pmatrix}. \quad (1.27)$$

Note that the inverse quench is associated with a matrix $\Gamma[\omega^{\text{out}} \rightarrow \omega^{\text{in}}]$ with off-diagonal entries of opposite signs.

On the other hand, the fundamental matrices acting on $(\hat{A}, \hat{B}^\dagger)^T$ for the free evolution with

$$\hat{A}(t_0 + \tau) = \hat{A}(t_0) e^{-i\omega_k \tau} \quad (1.28)$$

(and similar for $\hat{B}$) are clearly $\phi(\tau) = \Omega(\omega\tau)$ with

$$\Omega(x) := \text{diag}(e^{-ix}, e^{ix}). \quad (1.29)$$

Since the time evolution is from right to left in multiplying fundamental matrices, the composition

$$\phi = \Gamma[\omega_2 \rightarrow \omega_1] \Omega(\omega_2 \tau) \Gamma[\omega_1 \rightarrow \omega_2] \Omega(\omega_1 \tau) \quad (1.30)$$

yields the matrix in equation (1.12) describing a single period of the square wave that starts with free evolution with $\omega_1 = \omega(U_1)$ for time τ , undergoes a quench to $\omega_2 = \omega(U_2)$ at time τ , and after another period of free evolution falls back to ω_1 .

Some algebra gives the following results for the entries of ϕ ,

$$|\beta_T|^2 = 4\mathfrak{A}_k^2 \mathfrak{B}_k^2 \sin^2(\omega_2 \tau) \quad (1.31)$$

$$\arg \beta_T = -\omega_1 \tau - \pi/2 \quad (1.32)$$

$$\begin{aligned} \alpha_T &= \mathfrak{A}_k^2 \cos(\omega_1 + \omega_2) \tau - \mathfrak{B}_k^2 \cos(\omega_1 - \omega_2) \tau \\ &\quad - i \left[\mathfrak{A}_k^2 \sin(\omega_1 + \omega_2) \tau - \mathfrak{B}_k^2 \sin(\omega_1 - \omega_2) \tau \right] \end{aligned} \quad (1.33)$$

$$\begin{aligned} &= \cos \omega_1 \tau \cos \omega_2 \tau - (\mathfrak{A}_k^2 + \mathfrak{B}_k^2) \sin \omega_1 \tau \sin \omega_2 \tau \\ &\quad - i \left[\sin \omega_1 \tau \cos \omega_2 \tau + (\mathfrak{A}_k^2 + \mathfrak{B}_k^2) \sin \omega_2 \tau \cos \omega_1 \tau \right] \end{aligned} \quad (1.34)$$

$$\arg \alpha_T = -\omega_2 \tau - \arctan[(\mathfrak{A}_k^2 + \mathfrak{B}_k^2) \tan \omega_2 \tau], \quad (1.35)$$

and in particular,

$$\text{Re } \alpha_T = \cos \omega_1 \tau \cos \omega_2 \tau - (\mathfrak{A}_k^2 + \mathfrak{B}_k^2) \sin \omega_1 \tau \sin \omega_2 \tau. \quad (1.36)$$

We can now write down the mode occupation after N periods by combining equation (1.36) with the result (1.16) above and find after simplification for the quasiparticle number spectrum:

$$\begin{aligned} |\beta_k(t=0)|^2 &= |\beta(N, \omega_1(k), \omega_2(k))|^2 = \\ &= \left[\frac{(\omega_1^2 - \omega_2^2) \sin(\omega_2 T)}{2\omega_1 \omega_2} \frac{(q_1 - q_2)^N - (q_1 + q_2)^N}{2q_2} \right]^2, \end{aligned} \quad (1.37)$$

where

$$q_1 := \Re \alpha_k(t_1) = \cos \omega_1 \tau \cos \omega_2 \tau - \frac{\omega_1^2 + \omega_2^2}{2\omega_1 \omega_2} \sin \omega_1 \tau \sin \omega_2 \tau, \quad (1.38)$$

$$q_2 := \sqrt{q_1^2 - 1}. \quad (1.39)$$

As argued above, to find the fastest growing resonant cases for $N \gg 1$ we should find the global maxima of $\Re \alpha_k(t_1)$ as a function of k . This is non-trivial due to the oscillatory form of this function.

Resonances for Large Driving Amplitudes

Parametric resonance for the strongly driven, classical problem has been studied numerically for a variation of the scattering length in [Cairncross and Pelster, 2014] and analytically for a variation of the trap in [Garcia-Ripoll et al., 1999].

Here we derive some analytic results for large variations of the scattering length within the linear theory. Note that this may drastically increase the condensate depletion and will eventually lead to violation of the assumed linear theory. However, even when a resonant mode is strongly excited, the particle number can be insignificant with respect to the total depletion for a system with many modes.

Fast growing, nonperturbative parametric resonances have been suggested to cause preheating in the reheating process of the inflationary universe [Kofman et al., 1994].

In view of equation (1.33) one may consider interaction strengths such that for particular values of $k = k_{sr}$ (where the subscript stands for “super-resonant”) we have both $\sin \omega_1(U_1, k_{sr})\tau = \pm 1$ and $\sin \omega_2(U_2, k_{sr})\tau = \pm 1$. There is an infinite, discrete set of such wave numbers together with step heights $h_{sr} := U_2/U_1$ for any initial value of the interaction strength U_1 such that these two equations are simultaneously satisfied. Rewriting $\Re \alpha_T = q_1 = (\cos \omega_1 \tau \cos \omega_2 \tau - \sin \omega_1 \tau \sin \omega_2 \tau) - 2\mathfrak{B}_k^2 \sin \omega_1 \tau \sin \omega_2 \tau$, we then see that both the first part (which can also be written as $\cos(\omega_1 + \omega_2)\tau$) and the second part are extremized with the same sign, if $\mathfrak{B}_k$ is assumed to be constant. Note that these conditions on ω_1 and

ω_2 are equivalent to having all phases dropping out of the matrix ϕ , which is can be seen from equations (1.35, 1.32).

The solutions can be parametrized by $(a_1, a_2) \in \mathbb{N}^2$ with $a_1 \neq a_2$ as

$$\omega_{1/2} = \omega_D(a_{1/2} + 1/2), \quad (1.40)$$

where we have defined the *driving frequency* $\omega_D := \pi/\tau$ ¹. We parametrize the Bogoliubov dispersion (1.5) as $\omega_{1/2}^2 = c_{1/2}^2 k^2 + \epsilon^2 k^4$, which implies $\epsilon = \hbar^2/4m^2$ and $c_{1/2}^2 = U_{1/2}n/m$, and we define $\rho_{1/2} := \frac{4\epsilon^2\omega_{1/2}^2}{c_1^4}$, which depend on the integers a_1 and a_2 through the frequencies (1.40). Then we can calculate that

$$k_{sr} = \frac{c_1}{\sqrt{2}\epsilon} \sqrt{\sqrt{1+\rho_1}-1}, \quad (1.41)$$

$$h_{sr} = \frac{1}{2} \left(1 - \sqrt{1+\rho_1} + \frac{\rho_2}{\sqrt{1+\rho_1}-1} \right). \quad (1.42)$$

In these super-resonant cases the result (1.37) at final time $t = 0$ simplifies drastically to

$$|\beta_{k,sr}|^2 = \frac{1}{4} \left(\left(\frac{\omega_2}{\omega_1} \right)^N - \left(\frac{\omega_1}{\omega_2} \right)^N \right)^2. \quad (1.43)$$

which is an expression depending on k and h and provides an upper bound for particle production in the general, not super-resonant case, $k \neq k_{sr}$ or $h \neq h_{sr}$. Taking into account the nonlinear dispersion relation, this upper bound increases rapidly for decreasing k . This has the consequence that the super-resonance peaks at k_{sr} are not necessarily indicating the globally maximal particle production in the non-linear case. If k_{sr} is far in the nonlinear (free particle) regime of the dispersion relation it may happen that a mode $k \ll k_{sr}$ corresponding to a local maximum of $|\Re\alpha_T|$ grows faster even though the super-resonance condition (1.40) is not fulfilled for this wave number.

Furthermore, the above assumption that $\mathfrak{B}_k$ does not depends on k and h is just an approximation, and at k_{sr} the derivative dq_1/dk is not exactly equal to zero. The ratio of the produced particles to the super-resonant k -dependent maximum, $|\beta_k/\beta_{k,sr}|^2$, reaches its maximum 1 precisely at k_{sr} . However, $\beta_{k,sr}$ is a decreasing function with k varying slowly

¹As on page 17, the driving frequency is the angular frequency of the periodic modulation signal, since the period length for rectangular modulation is 2τ .

with respect to the oscillations in $|\beta_k|$. The actual maximum of $|\beta_k|$ is thus shifted to lower values of k by an amount of the order of the peak width. Thus, k_{sr} still indicates the *same* resonant peak in this case, just not the center.

The super-resonant case for $a_1 = 0$, $a_2 = 2$ is shown in figure (1.1). Here, the solid black line is the prediction for $|\beta_k|^2$ for ten steps obtained by multiplying numerically the corresponding phase-evolving quench matrices obtained from a QFT in curved background approach as outlined in [Weinfurtner et al., 2007]. The green, dotted line is the above exact solution (1.37), where all quench matrices are identical. The curves agree exactly, as they should. Indeed it can be shown that the first approach in [Weinfurtner et al., 2007] can be transformed by matrix decompositions such that all intermediate phase dependencies cancel, leading the same analytical result as the more straightforward approach from within Bogoliubov theory shown here.² Also plotted is the predicted maximal production (1.43) as a function of k and a vertical line at k_{sr} given in equation (1.41).

Corrections for Low-Amplitude Parametric Driving

Of the greatest practical importance is however the following resonance, which is not an exact “super-resonance”. If the interaction strength is only varied slightly, exponential growth is still obtained for large N . It is clear that the super-resonance condition (1.40) cannot be satisfied for small but finite variations. It can be shown that as the particle production tends to zero in the limit of vanishing variation of the interaction strength, the parametric resonance actually approaches a super-resonance in the sense that equation (1.43) is still correct up to sufficiently high order in the small variation. Further, an approximate expression for the position of the resonances can be derived which is of the form of a frequency matching condition:

$$\omega_1(k_r) + \omega_2(k_r) = \omega_D. \quad (1.44)$$

This is a correction to the well-known result that the driving frequency should be double the frequency of the mode which is to be excited for parametric resonance [Faraday, 1831, Rayleigh,

²We decided not to include the (long) proof.

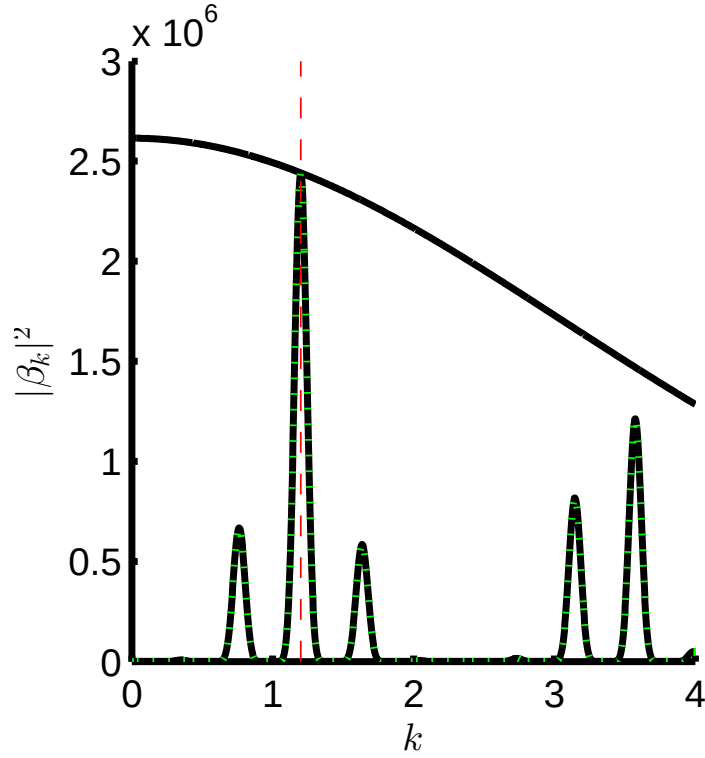


Figure 1.1.: Prediction for the super-resonant particle production solution parametrized by $(a_1, a_2) = (0, 2)$ for $\epsilon = 0.1$ and $N = 10$ with $c_1 = 1$, yielding $c_2 = 5.034$. (See Chapter A.1 for the dimensionless rescaling.). Several, wide, unstable regions show growth (black/green). The prediction of the maximum value of $|\beta_k|$ (the top line) is exact, and the formula for the peak position (red vertical) is very accurate (slightly shifted to the right, invisible here).

1887]. It is emerging here for the analytical results for the square wave. However, note that we found by numerical study that it generalizes as expected to the case of sinusoidal modulations, treated in the next Section. Smooth modulations are more interesting than rectangular modulations, as they avoid the introduction of high frequency harmonic contributions and are possibly more easily accomplished experimentally, since sudden changes of e.g. magnetic fields are a theoretical abstraction.

Despite the frequency matching condition (1.44) being equivalent to a fourth order polynomial

in k_r^2 , this can be solved to obtain

$$k_r = \omega_D \sqrt{\frac{c_1^2 + c_2^2 - 2\sqrt{c_1^2 c_2^2 + \epsilon^2 \omega_D^2}}{(c_1^2 - c_2^2)^2 - 4\epsilon^2 \omega_D^2}}. \quad (1.45)$$

In the linear case this reduces to

$$k_r = \frac{\omega_D}{c_1 + c_2} = \frac{\omega_D}{c_1} \frac{1}{1 + \sqrt{h}}. \quad (1.46)$$

We see that these corrections appear already at first order of the small amplitude since $\frac{1}{1+\sqrt{h}} \approx 1/2 - (h-1)/8$.

Knowledge of these formulas is useful for a precise numerical treatment to align the resonance exactly with modes which are represented on the numerical grid, any may also turn out to be useful for future experiments.

Application to Sinusoidal Driving

The numerical integration of the differential system (1.22) for $\text{Re } \alpha_T$ show great agreement of the case of sinusoidal variation with $4/\pi$ the amplitude of the rectangular steps in particular in the phononic regime. This means that the fundamental fourier mode of the step is dominating the growth behaviour for the first peak.

This is shown in figure (1.2) comparing $|\text{Re } \alpha_T| - 1$ for the case of sinusoidal driving with square waves of different amplitude. The dimensionless driving frequency $\omega_D = 0.2$ and driving is relatively strong with an amplitude of $\pm 33\%$ around the mean interaction strength, broadening the peaks considerably. We use units in which the speed of sound $c = \sqrt{2}/2$, described in Chapter (A.1).

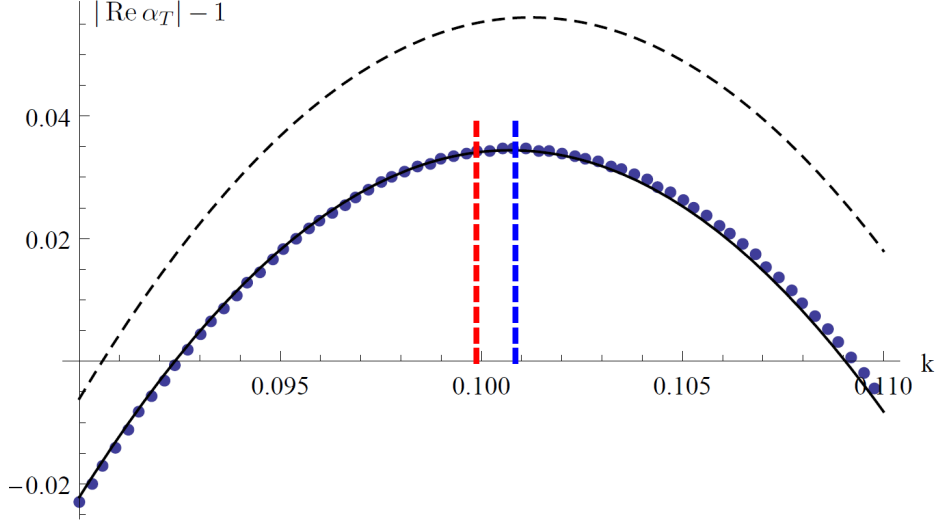


Figure 1.2.: The exact, numerically integrated results for $|\operatorname{Re} \alpha_T| - 1$ from sinusoidal driving are represented by the blue dots for various values of k around the main resonance. Positive values indicate exponential growth whereas negative values do not grow but oscillate. In comparison we show the analytical result for a square wave modulation with the same amplitude as the black dashed line. If we correct the amplitude of this modulation to value smaller by a factor of $\pi/4$, we approximate the numerics for the sine well with the square wave analytics (black solid line). Also shown is the prediction of the maximum for the square wave by the frequency matching condition $\omega(k, U_1) + \omega(k, U_2) = \omega_D$ (blue dashed line) in comparison to a naïve solution of $\omega(k, \bar{U}) = \omega_D/2$ (red dashed line), showing that the first approach is more accurate.

2. Experimental Proof of Nonclassicality?

Motivated from quantum optics studies three kinds of inequalities were utilized in recent BEC experiments, with the goal to determine nonclassicality in atom optics experiments, namely sub-Poissonian statistics [Kheruntsyan and Drummond, 2002, Ögren et al., 2009, Jaskula et al., 2010, Jaskula et al., 2012, Wasak et al., 2014, van Frank et al., 2015], and intensity [Olsen et al., 2002, Marino et al., 2008, Buchmann et al., 2010, Kheruntsyan et al., 2012, Wasak et al., 2014, de Nova et al., 2014, de Nova et al., 2015b, de Nova et al., 2015a, Boiron et al., 2015] and mode [Campo and Parentani, 2005, Busch and Parentani, 2013, Busch and Parentani, 2014, Finazzi and Carusotto, 2014, Busch et al., 2014, Steinhauer, 2015, Steinhauer, 2014, Steinhauer, 2016] Cauchy-Schwarz inequalities (CSIs). Among these three inequalities sub-Poissonian statistics is the most accessible variable, as it can be obtained directly from the normalised number difference variance, also referred to as the two-mode variance (TMV). The intensity CSI involves *normally* ordered density-density correlations of two symmetrically occupied modes, and is violated when the normally ordered cross-correlations exceed the normally ordered auto-correlations, see eq. (2.2). In [Kheruntsyan et al., 2012] it was argued that the normally ordered density-density correlations are accessible in time-resolved time-of-flight (TOF) measurements. The mode Cauchy-Schwarz inequality is a comparison between *anomalous* and mode density. A direct measurement of the anomalous density is not possible, but recently an indirect measurement of it has been suggested [Steinhauer, 2015, Steinhauer, 2016].

As we shall see, from all of the above mentioned criteria *only* the mode CSI is *in principle* a sufficient measure of nonclassicality in the sense of ruling out our classical reference. We also show that given some stronger assumptions, i.e. the validity of the approximate

quantum theoretical model (within the Bogoliubov approximation the quantum states for the excitations are Gaussian), all of the three criteria are mathematically equivalent, and since the mode Cauchy-Schwarz inequality is violated if and only if the state is nonseparable [Busch, 2014], all three of them can equally well facilitate as entanglement criteria. Nevertheless we show explicitly, when it comes to the experimental realization of the above mentioned criteria, *none* of them are sufficient measures of nonclassicality in the experimental set-up under consideration here.

2.1. Number Correlation-based Nonclassicality criteria from quantum optics

In quantum optics an important class of observables is provided by absorbing photodetection. As a case in point we consider monochromatic light emitted from a point source and photo detectors with no dead time that detect light of a specific wave vector. In the semiclassical theory of atom-light interactions [Bohr et al., 1924b, Bohr et al., 1924a] the joint click rates of a single or several photodetectors are directly proportional to the moments of mode intensities. In the theory of the quantized field the intensity I_a of a mode a is represented by the photon number operator $\hat{n} = \hat{a}^\dagger \hat{a}$, and the joint click rates are proportional to *normally and time ordered* moments of this operator [Vogel and Welsch, 2006]; e.g. for m coincident measurements at equal time and position they are proportional to $\langle (\hat{a}^\dagger)^m \hat{a}^m \rangle = \langle \hat{n}(\hat{n} - 1) \dots (\hat{n} - m + 1) \rangle$. The destructive measurement of photons results in decreased auto-correlations, while the classical reference assumes a “non-destructive” measurement of waves resulting in $\langle n^m \rangle_d$, where $n = I$ is the (fluctuating) mode intensity. For example consider the observation of intensity correlations $C(\tau) = \mathbb{E}(I(t)I(t + \tau))$ of continuously emitted light (i.e. in a stochastic steady-state) from a fluorescing atom at two subsequent times separated by τ as recorded by a single detector (we use the notation $\mathbb{E}(\dots)$ for mean values of observables as measured in the laboratory). If the density-density correlations are increasing with $\tau \geq 0$, we can rule out the classical model because the Cauchy-Schwarz theorem would always imply $dC/d\tau(0) \leq 0$ [Vogel and Welsch, 2006]. However, the observation of $dC/d\tau(0) > 0$, known as

photon antibunching, was reported in [Kimble et al., 1977]. This effect is genuinely nonclassical by definition because it is not understood within the classical reference. Within quantum theory, the observed data can be explained by the fact that single photons are arriving with a tendency of being separated from each other and the normally ordered correlator is strongly decreased. The criterion for quantum states allowing for the observation of $dC/d\tau(0) > 0$ can be formulated as the inequality

$$\langle \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \rangle < \langle \hat{a}^\dagger \hat{b}^\dagger \hat{b} \hat{a} \rangle, \quad (2.1)$$

where $\hat{a} = \hat{a}(t)$, $\hat{b} = \hat{a}(t + \tau)$, $t > 0$. It follows that this expression serves as a sufficient *nonclassicality criterion* for the quantum state in an experiment of the type outlined above.

The concept of nonclassical states and any corresponding criteria can be extended to the case of multiple detectors. In particular, let $|\alpha, \beta\rangle$ be a tensor product of coherent states for two modes a, b entering two detectors at different positions, and consider the measurement of coincident click rates, proportional to normally ordered correlators of $\hat{n}_a, \hat{n}_b$ in the quantum theory. Further, let us call states $\rho = \int d\alpha d\beta P(\alpha, \beta) |\alpha, \beta\rangle \langle \alpha, \beta|$ *P-classical* if their Glauber-Sudarshan P-representation $P(\alpha, \beta)$ has the properties of a classical (i.e. positive) probability distribution for the two complex mode amplitudes. Using the defining property that the coherent states are eigenstates of their corresponding mode annihilation operators, it is evident that one can reproduce any coincident click rate within the classical reference by using $P(\alpha, \beta)$ as the probability distribution for the complex classical mode amplitudes [Titulaer and Glauber, 1965, Mandel, 1986, Vogel and Welsch, 2006]. On the other hand, for *P-nonclassical* states without such a P-representation there should exist in principle a coincidence counting experiment falsifying the classical theory. Thus, in the case of measuring such counting rates in quantum optics, a state is classical if and only if it is P-classical. A sufficient criterion to establish P-nonclassicality of a state is similarly given by inequality (2.1), where now a and b are two different modes at equal time, as is proven by contradiction from the Cauchy-Schwarz theorem. This inequality is equivalent to

$$G_{a,b}^{(2,2)} > (G_{a,a}^{(2,2)} G_{b,b}^{(2,2)})^{1/2}, \quad (2.2)$$

for the special case that $G_{a,a}^{(2,2)} = G_{b,b}^{(2,2)}$. Here $G_{ab}^{(2,2)} \equiv \langle \hat{a}^\dagger \hat{b}^\dagger \hat{a} \hat{b} \rangle$ are the normally ordered correlators. We therefore refer to this criterion as the violation of the *intensity CSI*.

We now discuss the connection of the intensity CSIs and another correlation measure, the two-mode variance (TMV), also called the number squeezing parameter [Ögren et al., 2009, Buchmann et al., 2010], which is experimentally accessible by repeatedly measuring the intensity of the two modes. The TMV is defined as the normalized number difference variance

$$V = \text{Var}(I_a - I_b) / \mathbb{E}(I_a + I_b) \geq 0 \quad (2.3)$$

for two modes labelled a and b . Similar to referring to the case of a single variable with a variance smaller than its mean as sub-Poissonian, we refer to $V < 1$ as sub-Poissonian statistics in accordance with the literature. However V is sensitive to both the single-mode statistics and two-mode correlations. While $V = 1$ for the state $|\alpha, \beta\rangle$, in general neither uncorrelated nor Poissonian variables are necessary for $V = 1$ ¹. For the symmetric case, where $\mathbb{E}((I_a)^n) = \mathbb{E}((I_b)^n)$ for $n = 1, 2$, the TMV simplifies to

$$V = \frac{\mathbb{E}(I_a I_a) - \mathbb{E}(I_a I_b)}{\mathbb{E}(I_a)}. \quad (2.4)$$

In a *quantum theory* this can be written as

$$V = 1 + \frac{G_{a,a}^{(2,2)} - G_{a,b}^{(2,2)}}{\langle \hat{n}_a \rangle}, \quad (2.5)$$

so that it follows that $V < 1$ and a violation of the intensity CSI are equivalent, as was noted previously in [Kheruntsyan et al., 2012]. Note that since $V \geq 0$, equation (2.4) also proves that cross-correlations never exceed the *non-normally* ordered auto-correlations; the normal ordering is crucial for a violation of the intensity CSI. In a quantum theory, due to the non-zero commutator, the normal ordering reduces the density-density auto-correlations, such that $G_{a,a}^{(2,2)} = \langle \hat{n}_a^2 \rangle - \langle \hat{n}_a \rangle$, which allows for $G_{a,a}^{(2,2)} < G_{a,b}^{(2,2)}$.

For the BEC, the implication that P-nonclassical states can demonstrate nonclassical behavior is not generally true, as it is fundamentally based on the ability to measure normally ordered moments of intensity in the quantum theory while at the same time these are represented without normal order in the classical reference. We will see below that this is not the case in

¹An example are the binomially distributed, anti-correlated numbers of particles found in two non-overlapping regions in a box filled with an ideal gas. Simple examples with (positive) correlations also exist.

the BEC. Thus the criteria for nonclassical states from quantum optics based on establishing P-nonclassicality, such as the violation of the intensity CSI (2.2), are not *a priori* related to nonclassicality.

To further explore these issues we focus on the specific example of (parametrically) excited, strongly correlated two-mode number fluctuations in a BEC [Jaskula et al., 2012]. To determine the validity of the nonclassicality criteria for this system it is necessary to compare both the quantum and the corresponding semiclassical theories, as described in Sections 1.2 and 2.2 respectively.

2.1.1. Prediction for Mode Number Density

We are primarily concerned with the momentum-space observables, which are the expectation values of products of time-dependent real particle operators of the form $a(t > 0)$ and/or its conjugate, as these observables can be measured in current experiments, e.g. using the standard time-of-flight (TOF) method [Anderson et al., 1995, Davis et al., 1995]. In a TOF experiment one measures real particles rather than quasi-particles, and in the following we will be focussing on observables in the real particle basis [Shvarchuck et al., 2002]. Note, this is in contrast to most of the analogue gravity studies on similar subjects, which focus on the quasi-particles modes, e.g. [Barceló et al., 2011, Steinhauer, 2015, Busch and Parentani, 2013, Busch et al., 2014, Busch and Parentani, 2014]. Combining the interaction squeezing (1.3) with the parametric excitations for $t < 0$ (1.8) and the subsequent phase evolution, we have $\hat{a} = \lambda_k(t)^* \hat{A}^{\text{in}} + \gamma_k(t) \hat{B}^{\text{in}\dagger}$ and $\hat{b}^\dagger = \lambda_k(t) \hat{B}^{\text{in}\dagger} + \gamma_k^*(t) \hat{A}^{\text{in}}$. Because the Bogoliubov transformations form a group, the coefficients of the total transformation satisfy $|\lambda_k(t)|^2 - |\gamma_k(t)|^2 = 1$, and are given by

$$\lambda_k(t) = u_k^{\text{out}} \alpha_k e^{i\omega_k^{\text{out}} t} + v_k^{\text{out}} \beta_k e^{-i\omega_k^{\text{out}} t}; \quad (2.6)$$

$$\gamma_k(t) = u_k^{\text{out}} \beta_k e^{-i\omega_k^{\text{out}} t} + v_k^{\text{out}} \alpha_k e^{i\omega_k^{\text{out}} t}, \quad (2.7)$$

and a straightforward calculation shows that

$$\begin{aligned} |\gamma_k(t)|^2 &= (v_k^{\text{out}})^2 + |\beta_k|^2 + 2(v_k^{\text{out}})^2 |\beta_k|^2 \times \\ &\times \left(1 - \kappa_k \cos \left[2\omega_k^{\text{out}} t + \delta_k \right] \right), \end{aligned} \quad (2.8)$$

where $\kappa_k = [(1 + (v_k^{\text{out}})^{-2})(1 + |\beta_k|^{-2})]^{1/2}$ and $\delta_k = \arg \alpha_k - \arg \beta_k$.

Starting from a thermal initial state, the number of particles in mode $\mathbf{k}$ for $t > 0$ is given by

$$n_k(t) := \langle \hat{a}^\dagger \hat{a} \rangle = n_k^{th} + |\gamma_k(t)|^2 + 2n_k^{th} |\gamma_k(t)|^2. \quad (2.9)$$

Here n_k^{th} refers to the initial population when $U = U(t^{\text{in}})$. With expression (2.8) the depletion

$$\Delta = \sum_{\mathbf{k} \neq 0} n_k(t) \quad (2.10)$$

is when time averaged,

$$\begin{aligned} \overline{\Delta} &= \sum_{\mathbf{k}} \left[n_k^{th} + v_k^{\text{out}2} + |\beta_k|^2 \right. \\ &\quad + 2(n_k^{th} v_k^{\text{out}2} + n_k^{th} \beta_k^2 + v_k^{\text{out}2} \beta_k^2) \\ &\quad \left. + 4n_k^{th} v_k^{\text{out}2} \beta_k^2 \right], \end{aligned} \quad (2.11)$$

in particular containing the following three terms: the *thermal depletion* n_k^{th} which vanishes only for $T^{\text{in}} = 0$, the *depletion due to interactions* $v_k^{\text{out}2}$ which vanishes only for $U^{\text{out}} = 0$, and the *quasiparticle production* β_k^2 which vanishes only for $U = \text{const}$. Furthermore all three mutual dual products of these terms appear as well as the triple product, signifying mutual amplification of these processes. For large but finite volume it is possible to stay in the validity regime of the Bogoliubov theory $\Delta \ll N$ by reducing the scattering length sufficiently. Significant interactions are still possible by increasing the particle density. For the rest of this work, we assume that we are in this regime with $\Delta \ll N$.

The only other non-vanishing correlation containing two operators is

$$m_k(t) := \langle ab \rangle = \gamma_k(t) \lambda_k^*(t) (1 + 2n_k^{th}). \quad (2.12)$$

The modulus squared

$$|m_k(t)|^2 = |\gamma_k(t)|^2 (1 + |\gamma_k(t)|^2) (1 + 2n_k^{th})^2, \quad (2.13)$$

is referred to as the *anomalous* density. Although the anomalous density is not directly observable in section 2.3.3 we discuss a proposal [Steinhauer, 2015] to observe this quantity indirectly. As we shall see the anomalous density plays an important role in terms of establishing the nonseparability for the quantum fluctuations in a BEC.

2.1.2. Mode Number Correlations

The two-mode squeezed thermal state we are considering here is the exponential of a quadratic expression in the mode operators. For such Gaussian states, a finite temperature Wick theorem exists for mode operator moments in anti-normal, normal, and symmetrized order, respectively. Higher moments can be computed by simply summing over all possible pairings of second moments of the mode operators.

This immediately gives the normal ordered correlation functions, where for clarity we reintroduce the $\mathbf{k}$ -dependence, as

$$G_{\mathbf{k},\mathbf{k}'}^{(2,2)}(t) = \begin{cases} 2n_k^2(t) & \mathbf{k}' = \mathbf{k} \\ n_k^2(t) + |m_k(t)|^2 & \mathbf{k}' = -\mathbf{k} \\ n_k^2(t) & \text{else} \end{cases} \quad (2.14)$$

In our abbreviated notation, $G_{aa}^{(2,2)} = 2n_k^2(t)$ and $G_{ab}^{(2,2)} = n_k^2(t) + |m_k(t)|^2$. Then, the two-mode variance (2.5) is

$$V = 1 + \frac{n_k^2 - |m_k|^2}{n_k}. \quad (2.15)$$

Thus, we have sub-Poissonian statistics and violation of the CSI if and only if $|m_k|^2 > n_k^2$. This is an entanglement criterion which was first derived in the context of cosmological inflation [Campo and Parentani, 2005] and subsequently applied to the *phonons* of quenched and parametrically excited BECs in [Busch and Parentani, 2013, Busch et al., 2014]. The connection of entanglement to the violation of the CSI has been noted previously [Busch, 2014]. We can rewrite expression (2.15) as

$$V = \frac{n_k^{th}(1 + n_k^{th})}{n_k^{th}(1 + 2|\gamma_k|^2) + |\gamma_k|^2}, \quad (2.16)$$

and in particular simplify the condition $V < 1$ to obtain

$$|\gamma_k^2(t)| > n_k^{th}(T/2). \quad (2.17)$$

Taking the limit of vanishing interaction $U^{\text{out}} \rightarrow 0$ quasiparticles reduce to real particles and the term $|\gamma_k^2(t)|$ may be replaced by $|\beta_k^2|$ in (2.17). Then this expression agrees with the *phonon* entanglement criterion found in [Bruschi et al., 2013].

2.1.3. Relation to Mode Entanglement

We now give an independent (and short) derivation that (2.17) is a nonseparability criterion for the real particles, i.e. atoms, of opposite momenta.

For a given partition of the Hilbert space into each of the two modes and the rest of the system $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b \otimes \mathcal{H}_r$ we may ask if a product state $\rho = \rho_{ab} \otimes \rho_r$ is separable with respect to the first two spaces. This means by definition that the bipartite state can be written as a mixture of products (i.e. a convex sum), $\rho_{ab} = \sum_i p_i \rho_a^i \otimes \rho_b^i$ with $\sum_i p_i = 1$ and $p_i > 0$, and the subsystems' states ρ_m^i might be taken to be pure without loss of generality. If this is not possible one has a nonseparable or entangled state with respect to $\mathcal{H}_a \otimes \mathcal{H}_b$ [Werner, 1989].

A requirement for a separable state is that the partial transpose of the density operator is again positive semi-definite [Peres, 1996]. If this is not the case the state must be nonseparable. For continuous variable two-mode systems, like for the two modes a, b considered here, the implication of this sufficient nonseparability criterion for the covariance matrix is also necessary for nonseparability if the state is a Gaussian Wigner function [Simon, 2000]. A straightforward procedure to evaluate this entanglement criterion conveniently written in terms of moments of the annihilation and creation operators directly is to consider the determinant [Shchukin and Vogel, 2005]

$$D_5 = \begin{vmatrix} 1 & \langle \hat{a} \rangle & \langle \hat{b}^\dagger \rangle & \langle \hat{b} \rangle & \langle \hat{a}^\dagger \rangle \\ \langle \hat{a}^\dagger \rangle & \langle \hat{a}^\dagger \hat{a} \rangle & \langle \hat{a}^\dagger \hat{b}^\dagger \rangle & \langle \hat{a}^\dagger \hat{b} \rangle & \langle \hat{a}^{\dagger 2} \rangle \\ \langle \hat{b} \rangle & \langle \hat{a} \hat{b} \rangle & \langle \hat{b}^\dagger \hat{b} \rangle & \langle \hat{b}^2 \rangle & \langle \hat{a}^\dagger \hat{b} \rangle \\ \langle \hat{b}^\dagger \rangle & \langle \hat{a} \hat{b}^\dagger \rangle & \langle \hat{b}^{\dagger 2} \rangle & \langle \hat{b} \hat{b}^\dagger \rangle & \langle \hat{a}^\dagger \hat{b}^\dagger \rangle \\ \langle \hat{a} \rangle & \langle \hat{a}^2 \rangle & \langle \hat{a} \hat{b}^\dagger \rangle & \langle \hat{a} \hat{b} \rangle & \langle \hat{a} \hat{a}^\dagger \rangle \end{vmatrix}. \quad (2.18)$$

Here rows and columns have been reordered such that D_5 trivially splits into the product of two sub-determinants for our case,

$$D_5 = (n_k^2 - |m_k|^2)((n_k + 1)^2 - |m_k|^2). \quad (2.19)$$

The state is entangled iff $D_5 < 0$ [Shchukin and Vogel, 2005]. Since in general $|\langle ab \rangle|^2 < \langle n_a \rangle \langle n_b + 1 \rangle$ [Adamek et al., 2013, Finazzi and Carusotto, 2014] the second factor is always positive and we have simply $|m_k|^2 > n_k^2 \Leftrightarrow$ entanglement, completing the proof.

Since for any mixed separable state $|\langle ab \rangle|^2 \leq \langle a^\dagger a \rangle \langle b^\dagger b \rangle$, $|m_k|^2 > n_k^2$ implies nonseparability even for non-Gaussian states [Shchukin and Vogel, 2005, Hillery and Zubairy, 2006]. The violation of the mode Cauchy-Schwarz inequality

$$|\langle \hat{a}_k \hat{a}_{-k} \rangle|^2 > \langle \hat{a}_k^\dagger \hat{a}_k \rangle \langle \hat{a}_{-k}^\dagger \hat{a}_{-k} \rangle, \quad (2.20)$$

is thus sufficient for nonseparability in general, and equivalent to nonseparability for the two-mode squeezed Gaussian states considered here. For Gaussian states with coherent properties it is independent of entanglement [de Nova et al., 2015a, Busch and Parentani, 2014].

The intensity Cauchy-Schwarz violation (2.2) itself on the other hand does not imply nonseparability in general when the moments do not factorize as for Gaussian states. For example, $V = 0$ for (mixtures of) Fock states $|n\rangle \otimes |n\rangle$ with the same number of particles in mode a and b . Without the Gaussian factorization the breakdown of the intensity CSI as an entanglement criterion is expected.

We see from (2.16) that for the thermal state of the non-interacting system with $\gamma_k = 0$ the fluctuations are always super-Poissonian, $V = 1 + n_k^{th}$, and thus the state is separable. Increasing $|\gamma_k|$ due to quantum depletion or parametric excitations however leads to a decrease of V and sub-Poissonian statistics and nonseparability are possible.

For the interacting system in equilibrium, i.e. without parametric excitation, it can be shown that V as a function of k increases with decreasing wave number k . For $k \rightarrow 0$, $V = 1$ is reached for $k_B T = Un$, i.e. the temperature is of the order of the chemical potential μ of the Bose gas. *Here the atoms with opposite momenta are nonseparable already for all k due to interactions.* This effect is absent for the quasiparticles.

The term $|\gamma_k|^2$ on the left hand side of formula (2.17) appears in (2.9). Within (2.9) it may be interpreted as a quantum, ‘spontaneous emission’ term, comprising both quasiparticle production and quantum depletion. Note that for high temperatures $n_k^{th}(T/2) \gg 1$ Bogoliubov theory implies a spontaneous emission term $|\gamma_k^2(t)| \gg 1$ and entanglement when sufficiently strong correlations $V < 1$ are measured, but it also predicts that the spontaneous emission is insignificant compared to the amplification of thermal noise. In the next subsection we

show that the same measurable strong correlations $V < 1$ which imply entanglement in Bogoliubov theory are possible in a classical theory without a notion of entanglement. In this theory the spontaneous emission term is absent and only amplification of the thermal occupation occurs.

2.2. Classical Analysis

When quantum and thermal fluctuations are neglected, the mean-field dynamics of a Bose-Einstein condensate are well-described by the so-called Gross-Pitaevskii equation (GPE), given by:

$$i\hbar\partial_t\phi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(r) + U(t)|\phi|^2\right)\phi, \quad (2.21)$$

where $\phi(t, x) = \langle\hat{\Psi}(t, x)\rangle$ is the complex-valued macroscopic wave function and $V(r)$ is the trapping potential taken to be zero for the homogeneous case considered here. Formally the GPE can be obtained from the Heisenberg equation of motion $i\partial_t\hat{\Psi} = [\hat{\Psi}, \hat{H}]$ in the quantum theory and by a replacement $\hat{\Psi} \rightarrow \phi$ in the operator equation of motion, as is well known. For a more detailed derivation see for example [Castin, 2001].

A suitable classical Hamiltonian yielding the GPE from the equation of motion is given by the mean field energy functional [Pethick and Smith, 2001]

$$H[\phi] = \frac{1}{2} \int d\mathbf{r} \left(\hbar^2 \nabla\phi^* \nabla\phi / m + U(t) \int d\mathbf{r}' |\phi|^2 |\phi|^2 \right) \quad (2.22)$$

with the understanding that the complex field $\phi(x) \equiv (Q(x) - iP(x))/\sqrt{2}$. Indeed with this definition Hamilton's equations $\partial_t Q = \delta H / \delta P$ and $\partial_t P = -\delta H / \delta Q$ appear in the form $i\partial_t\phi = \delta H / \delta\phi^* = \{\phi, H\}$, and the right hand side of this expression amounts to the same formal manipulations as in the right hand side of the Heisenberg equation of motion $i\partial_t\hat{\Psi} = [\hat{\Psi}, \hat{H}]$. We consider the system to be in a classical thermal state of the canonical ensemble with probabilities for a field configuration ϕ given by $p[\phi] = \exp(-\beta H[\phi])$. As in the quantum case, we may linearize and diagonalize the theory for sufficiently low classical depletion $\Delta = \sum_{k \neq 0} \phi_k^* \phi_k$. The linear transformations to the classical quasiparticles (normal modes) are completely analogous, preserving the correspondence between the equations of

motion of the quantum and classical case. This similarity between the quantum and classical linear theory is well known for the common-place approach of linearizing *after* deriving the equations of motion, i.e. writing either $\hat{\Psi}(x, t) \rightarrow \phi_0(x, t) + \delta\hat{\phi}(x, t)$ in the quantum case and $\phi(x, t) \rightarrow \phi_0(x, t) + \delta\phi(x, t)$ in the GPE case (for the homogeneous time-dependent case considered here, $\phi_0(t)$ is constant in space). Thus, we obtain the equations of motion for the classical theory without further calculation by making a replacement

$$\hat{A}, \hat{B} \rightarrow A, B \quad (2.23)$$

in the corresponding equations from the quantum theory (1.9), where the classical quasiparticles are defined by a similar linear Bogoliubov transformation of Fourier modes of the field as in the quantum case,

$$a = \lambda_k^* A^{\text{in}} + \gamma_k (B^{\text{in}})^*, \quad (2.24)$$

where again we have set $\phi_{\mathbf{k}} = a$, with the coefficients γ_k and λ_k similarly given by (2.6) and (2.7). We identify the mode intensity $\mathbb{E}(I_a)$ with $\langle a^* a \rangle_{cl}$, and similarly for the intensity correlations. Within this classical treatment of the BEC, we find again by evaluating a Gaussian integral that $\langle A^* A \rangle_{cl} = n_{k,cl}^{th}$ and $\langle AB \rangle_{cl} = 0$ for the initial thermal state. However now the energy is equally partitioned over all the field modes,

$$n_{k,cl}^{th} = \frac{k_B T}{\hbar \omega_k} \quad (2.25)$$

in accordance with the high temperature limit of the Bose-Einstein statistics with vanishing chemical potential. The equipartition of energy is indeed observed in equilibrating micro-canonical simulations of the projected GPE [Davis et al., 2001, Davis et al., 2002]. Note that furthermore it has been argued there that the projected GPE at finite temperature provides indeed a (classical) theory of the highly occupied modes of an actual Bose-Einstein condensate. We do not rely on a physical interpretation of the classical theory of this sort; instead, we just use it as a tool providing a definite classical reference, to define and isolate the quantum effects.

2.2.1. Classical Mode Number Correlations

Using the Bogoliubov transformation (2.24) we obtain

$$n_{k,cl}^2 := (\langle a^* a \rangle_{cl})^2 = (2|\gamma_k|^2 + 1)^2 (n_{k,cl}^{th})^2; \quad (2.26)$$

$$|m_{k,cl}|^2 := |\langle ab \rangle_{cl}|^2 = 4(|\gamma_k|^2 + 1)|\gamma_k|^2 (n_{k,cl}^{th})^2. \quad (2.27)$$

Notice the absence of terms leading to the spontaneous generation of field fluctuations within this classical treatment of the excitations. It is also worth stressing that even in the absence of a modulation, $\beta_k = 0$, the thermal noise is correlated by the interaction term in the real particle basis, which contributes to the (thermal) depletion. However, for $T \rightarrow 0$ this depletion goes to zero in contrast to the quantum formulation. From equation (2.26) and (2.27) it is immediate that $|m_{k,cl}| < n_{k,cl}$. Hence the *mode CSI cannot be violated* in this classical theory. This is in agreement with the mathematical Cauchy-Schwarz theorem.

The Wick theorem for the evaluation of higher correlation functions now follows from Isserlis' theorem [Isserlis, 1918] directly. The fourth moments needed in expression (2.4) for the two-mode variance are $\mathbb{E}(I_a I_a) = \mathbb{E}(a^* a a^* a) = 2 \langle a^* a \rangle_{cl}^2$ and $\mathbb{E}(I_a I_b) = \langle a^* a b^* b \rangle_{cl} = \langle a^* a \rangle_{cl}^2 + |\langle ab \rangle_{cl}|^2$. (Note, comparing the classical with the quantum theory no corrections due to normal ordering are needed in order to apply Wick's theorem.)

2.3. Comparison between classical and quantum theory for specific observables

Finally we apply our findings to recent experimental procedures to detect sub-Poissonian statistics, intensity CSI and mode CSI. We demonstrate that *none* of these proposed experimental observables can establish the nonclassicality of the excitations in a BEC undergoing an arbitrary modulation of the interaction parameter. Below we discuss in depth two proposals that can be implemented using a TOF and / in-situ imaging technique of the condensate. In a TOF measurement the trap is switched off and the atoms fall due to gravity while expanding rapidly due to the non-zero velocity distribution of the

excitations in the BEC. Hence in a TOF experiment real space density fluctuations are mapped onto the atomic momentum space distribution. The motional states of the real particles carry information about the motional states of the original quantum gas, see for example [Shvarchuck et al., 2002]. Conversely, in-situ measurements involve a direct imaging of the trapped condensate [Wilson et al., 2015, Steinhauer, 2015, Steinhauer, 2016, Lahav et al., 2010].

2.3.1. Sub-Poissonian Statistics

Independent of the underlying theory the TMV, see equation (2.4), can be extracted experimentally via TOF and/or in-situ measurements. From a single experiment one can extract $I_a I_a$, $I_a I_b$ and I_a . By repeating the experiment and then averaging over the extracted quantities one can then get the corresponding expectation values. As pointed out above if the TMV is smaller than 1 the statistics of the process is referred to as sub-Poissonian.

Our classical reference predicts

$$V_{cl} = \frac{n_{k,cl}^{th}}{2|\gamma_k|^2 + 1} . \quad (2.28)$$

Note that V and V_{cl} are mathematically inequivalent expressions, but physically refer to the *same* observable. Thus we obtain sub-Poissonian statistics for

$$|\gamma_k^2(t)| > n_{k,cl}^{th}(T/2) - \frac{1}{2}, \quad (2.29)$$

within a completely classical treatment of small fluctuations in a BEC.

Comparing the quantum result (2.17) with the classical result (2.29), it appears that it is possible in both cases to produce sub-Poissonian statistics for a sufficiently low temperature and suitable modulation. We compare the time dependent value of V for a resonant mode undergoing periodic modulation for both the quantum and classical cases in the left column of Fig. 2.1. Here we plot the dependence of the experimentally measured values of V 's defined in (2.3) in the resonance mode for a square-wave modulation of the scattering length of a factor of 1.2 over 30 cycles for different initial temperatures. There are three important observations that can be made from these plots, which are true for both theories. First, V is

in general time-dependent due to the form of γ^2 given in Eq. (2.8). Second, for sufficiently long driving the oscillations become suppressed and V approaches zero. The oscillations in V for the quantum case also suggest that the entanglement criterion (2.17) is time-dependent. It should be noted that this refers to mode entanglement in contrast to particle entanglement. Third, the classical value V_{cl} is always below the quantum value V . This follows from comparing the criteria (2.29) and (2.17) and given that $n_{k,cl}^{th} < n_k^{th}$ at finite temperature. The physical explanation is that our classical reference is a wave theory and as such is missing the shot noise due to the discrete excitations (in this case atom numbers), i.e. the first term on the right hand side of $Var(\hat{n}_k) = \langle \hat{n}_k \rangle + \langle : \hat{n}_k \hat{n}_k : \rangle - \langle \hat{n}_k \rangle^2 = n_k + n_k^2$. The classical reference only contains the final term n_k^2 that has been associated by Einstein to the wave character of the atoms [Einstein, 1925]. The shot noise term is necessary for a (super-)Poissonian two-mode variance for low occupation numbers. To see this, we make use of an alternative form of expression (2.4), $V = (Var(I_a) - Cov(I_a, I_b))/\mathbb{E}(I_a)$ to bound V from above by $V \leq Var(I_a)/\mathbb{E}(I_a)$ for positive or vanishing correlations. Since classically the variance scales with the square of the occupation number, V will always be sub-Poissonian for low enough occupation numbers. Indeed, for equilibrium and vanishing interactions, (2.28) becomes $V_{cl} = n_{k,cl}^{th}$ showing the threshold is an occupation of unity.

We stress that the absence of shot noise in the classical theory is *not* always the cause of the obtained sub-Poissonian statistics. At high initial temperature $T \gg 1$ the shot noise becomes insignificant and the classical and quantum results approach each other. For strong enough driving, sub-Poissonian statistics is possible in both theories, even if the initial thermal state exhibits super-Poissonian fluctuations.

We conclude that a TMV smaller than 1, and / or sub-Poissonian statistics is *not* a sufficient nonclassicality criterion to rule out our specific classical reference.

2.3.2. Violation of Intensity Cauchy-Schwarz Inequality for Time-resolved TOF Measurements

As pointed out in (Sec. 2.1) the so-called violation of the intensity CSI, defined as auto-correlations exceeding cross-correlations, is only possible if the auto-correlations are normally ordered in the quantum theory or equivalently $I_a(I_a - 1)$ is measured instead of I_a^2 for the auto-correlations. If $V < 1$ a comparison of the cross-correlations with the auto-correlations in the reduced form $I_a(I_a - 1)$ appears in both the quantum and classical case. A distinction between the quantum theory and the classical reference as in coincidence counting experiments is then not available.

A time-resolved TOF method as proposed in [Kheruntsyan et al., 2012] is not a suitable detection scheme for this purpose. In the TOF method the atoms are released from the trap, hence the BEC is destroyed, and the wave description for the excitations breaks down. Collective excitations have been transferred to a finite number of atoms and hence independent of the nature of the collective excitations the measurement of the auto-correlations is destructive: the probability to subsequently measure two excitations with momentum k is proportional to $n_k(n_k - 1)$. In this sense the resulting violation of the CSI within a time-resolved TOF measurement of the density-density correlations is *not* a priori incompatible with a suitable classical description. It is instead equivalent to $V < 1$ and our discussion of the corresponding interpretation of this case applies directly to the results in [Kheruntsyan et al., 2012].

We conclude a time-resolved TOF measurement as suggested in [Kheruntsyan et al., 2012] is *not* a sufficient nonclassicality criterion for the excitations in a BEC.

2.3.3. Indirect Measurement of Violation of Mode Cauchy-Schwarz Inequality

The mode CSI could provide a way to establish the nonclassicality of the system. However, the anomalous density needs to be measured for this purpose. In [Steinhauer, 2015, Steinhauer, 2014] *in situ* density measurements were related to nonseparability criteria for the case of Hawking radiation which in the simplest case also reduce to a mode CSI between upstream

and downstream modes [Busch and Parentani, 2014]. A similar analysis was also given in [de Nova et al., 2015a]. The basic observables are the atom number densities at different positions in real space $\rho(\mathbf{r})$ measured for all $\mathbf{r}$ by an *in situ* imaging of the condensate.

The expectation value $\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{-\mathbf{k}} \rangle$, where $\hat{\rho}_{\mathbf{k}'} = \int d\mathbf{r} \hat{\rho}(\mathbf{r}) e^{-i\mathbf{k}'\mathbf{r}}$ and $\hat{\rho}(\mathbf{r}) = \hat{\Psi}(\mathbf{r})^\dagger \hat{\Psi}(\mathbf{r})$, can be obtained experimentally from the ensemble average $\mathbb{E}(\rho_{\mathbf{k}} \rho_{-\mathbf{k}})$ of the Fourier transform $\rho_{\mathbf{k}'} = \int d\mathbf{r} \rho(\mathbf{r}) e^{-i\mathbf{k}'\mathbf{r}}$ of the measured density $\rho(\mathbf{r})$ over different realisations (shots) of an identical experiment. Note that $\hat{\rho}_{\mathbf{k}}$ is not the number operator for mode $\mathbf{k}$ but a convolution $\hat{\rho}_{\mathbf{k}} = \sum_{\mathbf{p}} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{k}+\mathbf{p}}$ involving the (dimensionless) real particle annihilation and creation operators $\hat{a}_{\mathbf{k}} \equiv V^{-1/2} \int d\mathbf{r} \hat{\Psi}(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}}$, as can be easily verified by using $\hat{\Psi}(\mathbf{r}) = V^{-1/2} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}}$.

Making use of the Bogoliubov approximation (1.2) this is

$$\hat{\rho}_{\mathbf{k}} \simeq \sqrt{N}(\hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^\dagger). \quad (2.30)$$

Here we have assumed that the terms quadratic in the operators are bound by the total depletion. We can see immediately that $\hat{\rho}_{-\mathbf{k}} = \hat{\rho}_{\mathbf{k}}^\dagger$ and $[\rho_{\mathbf{k}}, \rho_{\mathbf{k}}^\dagger] = 0$. Thus $\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{-\mathbf{k}} \rangle = \langle \hat{\rho}_{\mathbf{k}}^\dagger \hat{\rho}_{\mathbf{k}} \rangle$ is a positive quantity and is approximately given by

$$\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{-\mathbf{k}} \rangle \simeq N \left[(\hat{a}_{-\mathbf{k}} \hat{a}_{\mathbf{k}} + h.c.) + (\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}} \hat{a}_{-\mathbf{k}}^\dagger) \right]. \quad (2.31)$$

In our previous notation and exploiting the symmetry of the state this reads $N(\hat{a}\hat{b} + \hat{a}^\dagger\hat{b}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger)$. In the quantum theory, the expectation value is thus

$$\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{-\mathbf{k}} \rangle = N(2\Re(m_k) + 2n_k + 1). \quad (2.32)$$

The behaviour of $m_k = \gamma_k \lambda_k^* (1 + 2n_k^{th})$ is determined by the complex factor

$$\begin{aligned} \gamma_k \lambda_k^* &= -|u_k v_k| (2|\beta_k|^2 + 1) \\ &+ \sqrt{|\beta_k|^2 + 1} |\beta_k| \left[2v_k^2 \cos(2\omega_k t + \delta_k) + e^{-i2\omega t - i\delta_k} \right]. \end{aligned} \quad (2.33)$$

(Note that $v_k < 0$ was used in the first term.) At times t_m such that $(2\omega t_m + \delta_k) \bmod 2\pi = \pi$, this reduces to

$$\gamma_k \lambda_k^* = -|u_k v_k| (2|\beta_k|^2 + 1) - \sqrt{|\beta_k|^2 + 1} |\beta_k| (2v_k^2 + 1), \quad (2.34)$$

a negative real number. Since all terms on the rhs of equation (2.34) appear with the same sign at t_m the term $|\gamma_k \lambda_k^*|$ is largest at this time. Thus, when measured at this particular time t_m , we can replace the real part by a minus sign,

$$\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{-\mathbf{k}} \rangle = 2N(n_k - |m_k|) + N. \quad (2.35)$$

We can then see that – assuming the quantum theory – at t_m the mode CSI violation (2.20) is equivalent to

$$\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{-\mathbf{k}} \rangle < N. \quad (2.36)$$

Keeping track of higher order terms shows that *one* condition for this analysis to hold is $\Delta \ll N/n_k$, which has to be compared to $\Delta \ll N$ for the validity of standard Bogoliubov theory, where Δ is the depletion of the condensate (2.10).

Note that we have $\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{-\mathbf{k}} \rangle = N$ in the limit of zero temperature, no driving and vanishing interactions due to the non-vanishing commutator. (The quantum noise causes the measured in-situ density to fluctuate). Thus, the observable consequence of entanglement in this experiment is a measured *suppression* of these fluctuations. The absence of quantum noise in any classical reference already indicates that such a threshold does not exist in our classical reference.

Indeed, at $t = t_m$ we obtain that

$$\mathbb{E}(\rho_{\mathbf{k}} \rho_{-\mathbf{k}}) = \langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle_{cl} = 2N(n_k - |m_k|), \quad (2.37)$$

hence it is also possible to obtain $\mathbb{E}(\rho_{\mathbf{k}} \rho_{-\mathbf{k}}) < N$. Very much like in the TMV case there are commutator terms only appearing within the quantum theory that make the observation imply a violation of the mode CSI. We plot the full time dependent predictions for this experiment in both the classical and the quantum theory in the right column of Fig. 2.1.

In summary, an indirect measurement of the mode CSI of the type suggested in [Steinhauer, 2015, Steinhauer, 2014] is *not* a sufficient non-classicality measure when applied to the case of excitations in a homogeneous parametrically excited BEC.

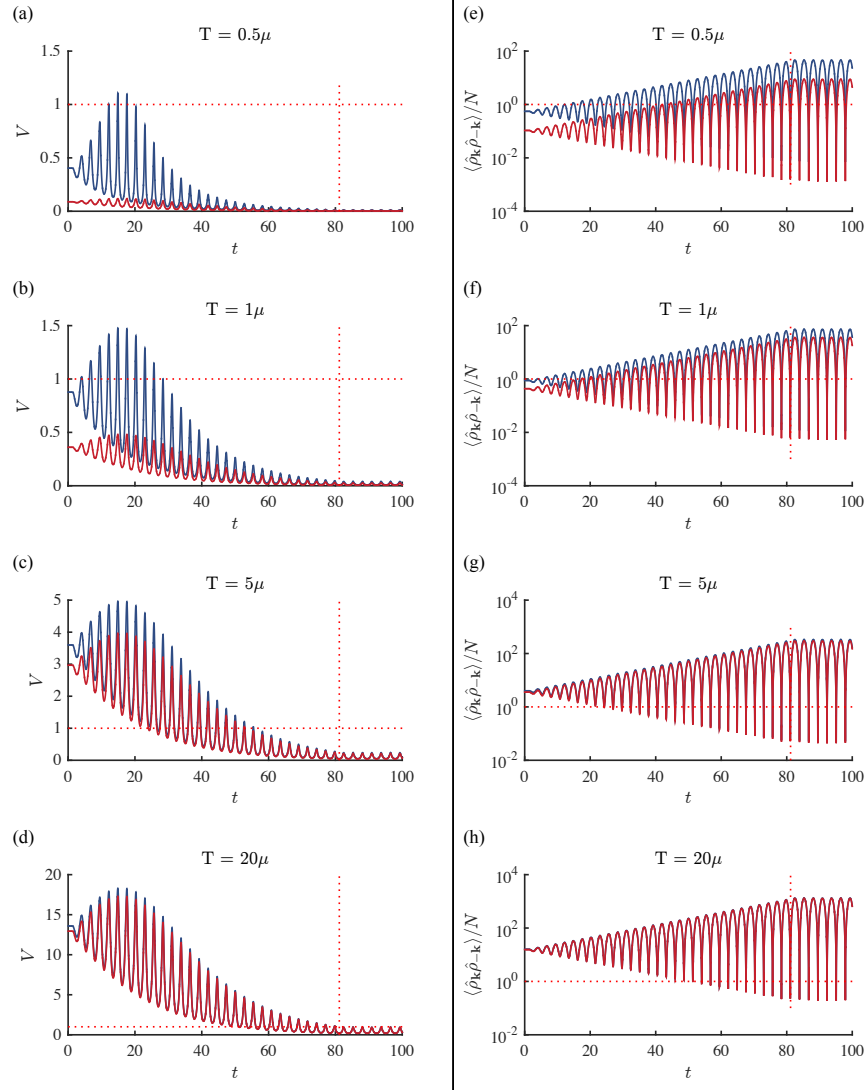


Figure 2.1.: Time dependence of the experimentally measured value of V as defined in (2.3) (left column) and $\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{-\mathbf{k}} \rangle$ (right column) in the quantum theory (blue) and classical reference (red) for first resonant mode at (a/e) $T = 0.5\mu$, (b/f) $T = 1\mu$, (c/g) $T = 5\mu$, and (d/h) $T = 20\mu$. The driving oscillation of the interaction strength, i.e. $U(t) = U_0(1 + 0.2F(t))$ with $F(t) = (1 - \text{sign}(\sin(\omega_D t)))/2$ for $\omega_D = \sqrt{5}$, in both cases is turned off after 30 periods as indicated by the (red) dotted vertical line. The (red) dotted horizontal line indicates in the column on the left (right) $V = 1$ ($\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{-\mathbf{k}} \rangle = N$). For $V < 1$ one speaks of sub-Poissonian number squeezing, and $\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{-\mathbf{k}} \rangle / N < 1$ has been proposed in [Steinhauer, 2015, Steinhauer, 2014] as an indirect measure of non-separability.

3. Conclusions of Part II

We have taken the viewpoint that nonclassical effects in the BEC are those that are incompatible with the results obtained using an ensemble of classical trajectories given by solutions of the GPE. For excitations in a parametrically excited BEC we showed that *observable* strong number correlations as indicated by $V < 1$ (related to P-nonclassicality and even nonseparability of atomic modes in the quantum theory) and an indirect measurement of the intensity CSI as suggested in [Steinhauer, 2015, Steinhauer, 2014] are compatible with this classical theory. Similarly, we argued that a violation of the intensity CSI in a time-resolved TOF measurement is compatible with the classical picture of an atomic cloud after destruction of the BEC. Although we considered the definite model of parametric creation of two-mode squeezing, we also argued above that in different set-ups one should also not automatically expect these number correlation-based observables to rule out a corresponding classical model, and possibly a quantum model with decoherence.

Nevertheless, in the context that the Bogoliubov theory is a valid approximation, a measurement of $V < 1$ (or equivalently a violation of the intensity CSI) is sufficient for P-nonclassicality and nonseparability, both of which are criteria that assess a given quantum state.

To date none of the quantum measures applied to analogue gravity studies are sufficient to theoretically single out the spontaneous process of amplified vacuum noise in terms of (measured) occupation numbers. We conclude that the experimental verification of the quantumness of the fluctuations remains an open challenge for future BEC experiments in general. For this purpose we propose that additional observables, including noncommuting ones, e.g. density *and* phase fluctuations, have to be measured. For example it is possible

to involve interference techniques where one measures the phase quadrature of quasi particles [[van Frank et al., 2014](#), [Schweigler et al., 2015](#), [Steffens et al., 2014](#)]. Returning to the particular set-up discussed above, a parametrically excited condensate, we would like to point out that such a system can be used to mimic models of cosmological particle production in table-top experiments [[Jain et al., 2007](#)]. As argued in this paper, even within highly controllable and repeatable BEC experiments one is for now facing a similar dilemma to the one of establishing the quantum origin of the fluctuations seeding our universe [[Maldacena, 2016](#)]. So far in both cases a suitable Bell-type experiment, that would for once and all resolve this issue, is absent.

Part III.

Simulations

4. PGPE and TWA Simulations: Theoretical Background

4.1. The PGPE

The Gross-Pitaevskii equation (GPE)

$$i\hbar\partial_t\phi = \left(-\frac{\nabla^2}{2m} + V(\mathbf{r})\right)\phi + g|\phi|^2\phi \quad (4.1)$$

appears at zero temperature as the semi-classical approximation of the coherent state path integral [Brown, 1994] of the many-body, second quantized system with contact 2-body interactions, thus determining the most probable coherent state starting from another state after some time evolution. The equation also appears as the effective equation governing the wave function of a single particle under the influence of the others coming from the Schrödinger equation, if a pure and factorized state is assumed [Leggett, 2006]. However, the applicability of the GPE can be extended to finite temperature, and even stimulated processes based on quantum noise can be included.

At finite temperature, an approximation connected with the semi-classical limit of non-equilibrium field theory yields the classical evolution with the GPE, with the additional property that the initial conditions are sampled according to the Wigner function of the initial state, which includes quantum noise effects. Observables are mapped to their Weyl symbol and evaluated on the GPE trajectories [Polkovnikov, 2010]. We follow this approach to derive the so-called Truncated Wigner Approximation (TWA) in Section 4.2.2 after introducing the Weyl mapping in Section 4.2.1.

On the other hand, if the occupation numbers are high, the quantum theory usually approaches a completely classical limit and quantum noise effects become irrelevant.

Even the Bose-Einstein distribution (for the phonons, i.e. at vanishing chemical potential) approaches the equipartition thermal occupation of the classical quadratic theory for high occupation numbers, i.e.

$$n_k = \frac{1}{e^{\beta\hbar\omega_k} - 1} \approx \frac{k_B T}{\hbar\omega_k} \quad (4.2)$$

in the high-temperature limit $\beta \rightarrow 0$. Other c-field techniques (where c may stand for *classical* as well as *complex*) than TWA [Blakie et al., 2008] can then be employed.

The region consisting of modes which are not highly occupied is typically (not too far from equilibrium) given by higher-energy modes, which may be neglected in what is called the Projected GPE approach [Davis et al., 2001, Davis et al., 2002]. For a single trajectory of such a simulation, which conserves energy and particle number despite the projection to a lower-energy space, a microcanonical statistical interpretation has to be employed, i.e. averages are to be computed as time averages.

If the cut-off of the mode region considered is sufficiently below the transition to low occupation numbers, the thermal cloud cannot be neglected. Its effects can, however, be approximated by driving noise and damping in the Stochastic GPE approach [Blakie et al., 2008].

Independently, we can arrive at the projection operation as a generally useful numerical tool. Since the GPE is nonlinear, higher frequencies appear immediately from an initially band-limited field, coupling all modes up to infinity. A field represented on a finite grid is already band-limited. After evaluation of a nonlinear term, higher frequencies than the Nyquist limit will be interpreted as lower frequencies causing an aliasing artefact. It is thus advantageous to evaluate the nonlinearity on a larger grid that can represent the shorter modes which are appearing (it would have to be three times as large in momentum space for a ϕ^3 term), and then project out the high frequencies at every time step. The projection of the PGPE methodology may thus be used in other numerical techniques that are based on solving the GPE [Jain, 2007], and we will include a projector even for TWA simulations.

4.2. Truncated Wigner Approximation

The most interesting aspect about TWA simulations [Sinatra et al., 2002, Polkovnikov, 2010, Gardiner and Zoller, 2000] is that for short enough times, the exact *quantum* expectation values are computed by averaging the observables' Weyl symbols over samples from the Wigner representation of the quantum state. In the common approach, the quantum theory is rewritten in terms of the Wigner functional, and then the evolution equation for the Wigner functional is approximated by dropping higher derivatives and using stochastic calculus to trade the functional integro-differential equation for a differential equation for sample paths. It is well known that this yields classical fields that have to be sampled from the initial Wigner functional and evolve according to the GPE [Dalton et al., 2014]. Symmetrized averages of field operator products are then calculated by averaging moments of the classical field over the sample trajectories.

Other approaches to understand the TWA include expressing the von-Neumann equation in functional form after the Weyl mapping described below with a subsequent expansion of the Moyal bracket. Using the fact that the so obtained classical equations of motion are those of a Hamiltonian system where the Liouville theorem holds, it follows that averages at later times can then be calculated by sampling at an earlier time [Polkovnikov, 2010].

Here, we chose as a third approach to derive the TWA from a path integral representation of the non-equilibrium dynamics. This avoids the use of stochastic calculus and instead allows for the use of popular and powerful tools developed in the context of quantum field theory. It also allows for deriving corrections to TWA [Polkovnikov, 2003]. We will start following [Polkovnikov, 2013] after developing the necessary phase space concepts in a form suitable for our purposes. Together with some explicit proofs that are filled in, this forms a pedagogical introduction to the work of Polkovnikov. We then point out some discrepancies arising from too formal calculations, but find a more precise treatment too complicated to fully include it here. Interestingly, when approaching the problem more mathematical with a stationary phase approximation than physically with assuming the smallness of a particular field a priori as in [Polkovnikov, 2013], we already find a generalisation of TWA at the

semiclassical level.

4.2.1. Weyl Ordering and Wigner Representation

In this section and the following one we are suppressing mode-labelling indices and treat single mode systems only. The generalization to multiple modes is straightforward by means of the tensor product; for fields in real space with continuous index we rescale the fields to be dimensionless and discretize as $\int d^3x \psi^\dagger(x) \psi(x) =: \sum (\psi_x \sqrt{d^3x})^\dagger (\psi_x^\dagger \sqrt{d^3x})$.

To define a particular operator $\leftrightarrow$ c-number correspondence we introduce the *Weyl symbol* $O_W(\alpha, \alpha^*)$ (or *Wigner-(Weyl) transform*) of an operator $O(a, a^\dagger)$ as

$$O_W(\alpha, \alpha^*) = \frac{1}{2} \int d^2\beta \langle \alpha - \beta/2 | O(a, a^\dagger) | \alpha + \beta/2 \rangle e^{\beta^* \alpha/2 - \beta \alpha^*/2}, \quad (4.3)$$

where the integration measure is defined as

$$d^2\beta := \frac{d\text{Re}(\beta) d\text{Im}(\beta)}{\pi}, \quad (4.4)$$

and the coherent states are defined according to the convention with unit normalisation

$$\langle \alpha | \alpha \rangle = 1, \quad (4.5)$$

equivalent to defining them to be generated by action of the displacement operator $D(\alpha) = e^{\alpha a^\dagger - \alpha^* a}$ on the vacuum. This implies the scalar product

$$(|\alpha\rangle)^\dagger |\beta\rangle \equiv \langle \alpha | \beta \rangle = e^{\beta^* \alpha} e^{-|\beta|^2/2 - |\alpha|^2/2}. \quad (4.6)$$

One can then show that [Brown, 1994]

$$\int d^2\gamma |\gamma\rangle \langle \gamma| = 1. \quad (4.7)$$

Note that there is also a common convention with un-normalized coherent states $|\widetilde{\alpha}\rangle := e^{|\alpha|^2/2} |\alpha\rangle$, which removes the second exponential on the right hand side of the scalar product (4.6) and restores analyticity of $|\widetilde{\alpha}\rangle$ in α and of $(|\widetilde{\alpha}\rangle)^\dagger$ in α^* , the latter of which we conveniently call $\langle \widetilde{\alpha^*}|$ instead of $\langle \widetilde{\alpha}|$ [Brown, 1994] to make the explicit that this bra-vector

is independent of α . A disadvantage of the second convention is that the resolution of identity (4.7) has to be modified. However, since $|\widetilde{\alpha}\rangle = e^{\alpha a^\dagger} |0\rangle$, it is obvious that

$$a^\dagger |\widetilde{\alpha}\rangle = \partial_\alpha |\widetilde{\alpha}\rangle \quad (4.8)$$

(we employ the Wirtinger calculus for the partial derivatives with respect to α and α^*), which implies the more complicated identity

$$a^\dagger |\alpha\rangle = e^{-|\alpha|^2/2} \partial_\alpha (e^{|\alpha|^2/2} |\alpha\rangle). \quad (4.9)$$

In further calculations, with the help of the resolution of identity, Gaussian integrals that appear can often be avoided. For example we can see the following Lemma,

$$\int d^2\beta e^{x(-|\beta|^2/2 + \beta^*(\alpha - \gamma) - \beta(\alpha^* - \gamma^*))} = \frac{2}{x} e^{-2x|\alpha - \gamma|^2}. \quad (4.10)$$

by writing $\alpha' = \alpha - \gamma$ and the integrand as $\langle -\sqrt{2x}\alpha' | \beta \sqrt{\frac{x}{2}} \rangle \langle \beta \sqrt{\frac{x}{2}} | \sqrt{2x}\alpha' \rangle e^{2x|\alpha'|^2}$ and resolve the inner projector to an identity when integrating over $\int d^2\beta = 2x^{-1} \int d^2(\beta\sqrt{x/2})$.

The Weyl symbol of a symmetrized product of ladder operators is simply given by replacing $a \rightarrow \alpha$, $a^\dagger \rightarrow \alpha^*$, as can be shown inductively. It is not difficult to confirm from the definitions that the Weyl symbol of the identity operator is equal to one; and scalar multiplication is clearly preserved, $x1_W = x$. The sum is preserved, too, and it is thus sufficient to consider monomials only. The following observation is crucial for continuing with the proof. A symmetrized monomial operator with n factors can be expressed as the sum of a symmetrized operator of $n - 1$ factors once multiplied from the right and once multiplied from the left with either $a^\dagger$ or a . For example, the operator $a^\dagger a + a a^\dagger$ is symmetric, and from it we can construct the symmetric $(a^\dagger)^2 a + a(a^\dagger)^2 + 2a^\dagger a a^\dagger$ by multiplying with $a^\dagger$ once from the left and once from the right and adding the results. Note that the *same* operator can also be expressed as $4((a^\dagger)^2 a + a(a^\dagger)^2 + a^\dagger a a^\dagger)/3$, which is four times the standard symmetrization of $(a^\dagger)^2 a$ defined by summing all permutations. The equivalence is seen by using $2(a^\dagger a a^\dagger)/3 = ((a^\dagger)^2 a + a(a^\dagger)^2)/3$. Many other equivalent expressions clearly exist (such as $2((a^\dagger)^2 a + a^\dagger a a^\dagger)$). In this sense, the symmetric representation of an operator is not unique. Here, by symmetric we essentially mean palindromic. It becomes unique by e.g. enforcing the inductive construction or by using the permutation prescription. For the purpose of

obtaining the Weyl symbol all these three different palindromic representations are valid as a starting point for the rule to replace $a \rightarrow \alpha$, $a^\dagger \rightarrow \alpha^*$ “for symmetrically ordered operators”. This rule is obviously not sensitive to the precise version of the symmetric ordering as long as the coefficients sum up to the same number (here 4). In the present example every one of the three expressions yields $4(\alpha^*)^2\alpha$. It may be conjectured that any palindromic rewriting of the same operator has the required “symmetry” property for the replacement rule for obtaining the Weyl symbol.

We consider one of the two cases explicitly, namely $O_n(a, a^\dagger) = a^\dagger O_{n-1} + O_{n-1} a^\dagger$. The other case is analogous. Here we may use the assumption that for $O_{n-1}(a, a^\dagger)$, taken to be symmetric, the Weyl symbol is obtained by replacement, $O_{n-1,W}(\alpha, \alpha^*) = O_{n-1}(a \rightarrow \alpha, a^\dagger \rightarrow \alpha^*)$. We need to show that $O_{n,W}(\alpha, \alpha^*) = \alpha^* O_{n-1,W}(\alpha, \alpha^*) + O_{n-1,W}(\alpha, \alpha^*) \alpha^* = 2\alpha^* O_{n-1,W}(\alpha, \alpha^*)$. Plugging in the first term $O = a^\dagger O_{n-1}$ into the definition (4.3) trivially gives, since $\langle \alpha - \beta/2 | a^\dagger = (\alpha^* - \beta^*/2) \langle \alpha - \beta/2 |$, the expression

$$\frac{1}{2} \int d^2\beta (\alpha^* - \beta^*/2) \langle \alpha - \beta/2 | O_{n-1}(a, a^\dagger) | \alpha + \beta/2 \rangle e^{\beta^* \alpha/2 - \beta \alpha^*/2}. \quad (4.11)$$

More interesting is the other term with $O = O_{n-1} a^\dagger$. We write

$$O_W = \frac{1}{2} \int d^2\beta \langle \alpha^* - \beta^*/2 | O_{n-1} a^\dagger | \alpha + \beta/2 \rangle e^{\beta^* \alpha/2 - \beta \alpha^*/2 - |\alpha|^2 - |\beta|^2/4} \quad (4.12)$$

$$= \frac{1}{2} \int d^2\beta \langle \alpha^* - \beta^*/2 | O_{n-1} \left(2\partial_\beta | \alpha + \beta/2 \rangle \right) e^{\beta^* \alpha/2 - \beta \alpha^*/2 - |\alpha|^2 - |\beta|^2/4} \quad (4.13)$$

$$= -\frac{1}{2} \int d^2\beta \langle \alpha^* - \beta^*/2 | O_{n-1} | \alpha + \beta/2 \rangle 2\partial_\beta e^{\beta^* \alpha/2 - \beta \alpha^*/2 - |\alpha|^2 - |\beta|^2/4} \quad (4.14)$$

$$= -\frac{1}{2} \int d^2\beta \langle \alpha^* - \beta^*/2 | O_{n-1} | \alpha + \beta/2 \rangle (-\alpha^* - \beta^*/2) e^{\beta^* \alpha/2 - \beta \alpha^*/2}. \quad (4.15)$$

This is the same result as for the first term with a different sign in front of the $\beta^*/2$. The corresponding integral thus cancels and what remains is indeed twice $\alpha^* O_{n-1,W}(\alpha, \alpha^*)$. This completes the proof.

Generally, in the Wigner representation, the expectation value $\langle O \rangle \equiv \text{Tr}(\rho O)$ of an operator O is the average of the associated Weyl symbol O_W

$$\langle O \rangle = \int d^2\alpha W(\alpha, \alpha^*) O_W(\alpha, \alpha^*) \quad (4.16)$$

weighted with the Wigner function

$$W(\alpha, \alpha^*) = \frac{1}{2} \int d^2\beta \langle \alpha - \frac{\beta}{2} | \rho | \alpha + \frac{\beta}{2} \rangle e^{\frac{1}{2}\beta^* \alpha - \frac{1}{2}\beta \alpha^*}, \quad (4.17)$$

which is itself the Weyl symbol of the state operator.

In the Schrödinger picture, the state and thus the Wigner function becomes time-dependent. On the other hand, in the Heisenberg picture, the Wigner function is evaluated using coherent states at the initial time (meaning eigenstates of the annihilation operator at initial time), and time-independent. Similarly, these initial coherent states are used for the calculation of the Weyl symbol of the observables for the formula (4.16) to hold. These operators have evolved in time, such that in practice to evaluate the matrix elements the time evolution operator appears for the evaluation of the matrix elements. In the next section, we prove that the TWA method is related to the semiclassical approximate solution to this problem. The statement (4.16) is going to be proven as a special case for vanishing evolution time.

The particular form of the expression (4.17) for the Wigner function as well as the Weyl transform (4.3) is of great use for us, but it is not commonly found in the literature despite in the work of Polkovnikov¹. The equivalence to the commonly used definition as the Fourier transform of the Wigner characteristic function χ_W [Gardiner and Zoller, 2000, Walls and Milburn, 2007, Agarwal, 2012],

$$W(\alpha, \alpha^*) = \int d^2\beta \chi_W(\beta, \beta^*) e^{\beta^* \alpha - \beta \alpha^*} \quad (4.18)$$

$$\chi_W(\beta, \beta^*) = \text{Tr}(\rho e^{\beta a^\dagger - \beta^* a}), \quad (4.19)$$

or the more similarly appearing original definition of Wigner, which itself is equivalent to (4.18) [Gardiner and Zoller, 2000],

$$W(q, p) = \frac{1}{\pi \hbar} \int dy \langle q + y | \rho | q - y \rangle e^{-2iyp/\hbar} \quad (4.20)$$

is not immediately obvious.² However, making use of the P-representation, we only need to

¹Polkovnikov partly also uses the unnormalized coherent states convention [Polkovnikov, 2010]. Note that in [Polkovnikov, 2013] the factor of 1/2 in front of definitions (4.17, 4.3) is erroneously missing.

²We remark that for the pq -form (4.20) the proof of (4.16), i.e. that the the Weyl symbol averaged with the Wigner function becomes the expectation value is particularly simple [Polkovnikov, 2013].

show equivalence for (averages of) coherent states. In fact, equation (4.17) is equal to

$$W(\alpha, \alpha^*) = 2 \int d^2\gamma P(\gamma) e^{-2|\alpha-\gamma|^2}, \quad (4.21)$$

which is the representation of the Wigner function in terms of the P-function. Before we show this, note that since here π^{-1} is absorbed in the integration measure, our distributions (4.18, 4.21) are larger by a factor of π than in other sources [Gardiner and Zoller, 2000] to ensure the normalization to unity *in addition to* factors of π for each integration measure in the formulas defining the distributions. Since both W and P are larger by the same factor, and there is one integration, our formula lacks a factor of π^{-1} compared to these sources, and $\int d^2\alpha W(\alpha, \alpha^*) = 1$. To show the (well-known) equivalence of (4.18) and (4.21), we first obtain the quantum characteristic function [Gardiner and Zoller, 2000], defined by

$$\chi(\beta, \beta^*) := \text{Tr}(\rho e^{\beta a^\dagger} e^{-\beta^* a}), \quad (4.22)$$

of the coherent state $|\gamma\rangle \langle\gamma|$ trivially as $\chi(\beta, \beta^*) = e^{\beta\gamma^* - \beta^*\gamma}$ and then get the Wigner function, according to (4.18), by Fourier transforming the Wigner characteristic function $\chi_W(\beta, \beta^*) = e^{-\frac{|\beta|^2}{2}} \chi(\beta, \beta^*)$ (this relation between the quantum and Wigner characteristic functions follows from the definitions using the BCH-formula). For the Gaussian integral we use Lemma (4.10) with $x = 1$ and get $2e^{-2|\alpha-\gamma|^2}$. Therefore, when a general state in (4.18) is expressed in the P-representation,

$$\rho = \int d^2\gamma P(\gamma) |\gamma\rangle \langle\gamma|, \quad (4.23)$$

we immediately find (4.21) as the P -average of the coherent state Wigner functions.

Finally we show equivalence of (4.21) and (4.17) similarly by calculating the Wigner function for $|\gamma\rangle \langle\gamma|$ from (4.17) as

$$W(\alpha, \alpha^*) = \frac{1}{2} \int d^2\beta \langle\alpha - \frac{\beta}{2}|\gamma\rangle \langle\gamma|\alpha + \frac{\beta}{2}\rangle e^{\frac{1}{2}\beta^*\alpha - \frac{1}{2}\beta\alpha^*} \quad (4.24)$$

$$= \frac{1}{2} \int d^2\beta e^{-\frac{|\beta|^2}{4} + \frac{\beta(\gamma^* - \alpha^*)}{2} - \frac{\beta^*(\gamma - \alpha)}{2} + \alpha^*\gamma + \gamma^*\alpha - |\gamma|^2 - |\alpha|^2} \quad (4.25)$$

$$= 2 \int d^2\frac{\beta}{2} \langle\gamma - \alpha|\frac{\beta}{2}\rangle \langle\frac{\beta}{2}| - (\gamma - \alpha)\rangle \quad (4.26)$$

$$= 2 \langle\gamma - \alpha| - (\gamma - \alpha)\rangle \quad (4.27)$$

$$= 2e^{-2|\gamma-\alpha|^2}. \quad (4.28)$$

In the second line we could alternatively have made use of the Lemma (4.10) with $x = 1/2$. It is clear that we find the result (4.21) for a general state (4.23), which completes the proof.

Since the Weyl symbol of an operator averaged with the Wigner function is the expectation value (c.f. (4.16)), it is the expectation values of symmetrically ordered operators that correspond to simple c-number moments of the Wigner function. Instead of dealing with the Wigner function itself and its time evolution, we will see below that one may effectively evolve samples from it (so-called trajectories) and carry out averages over trajectories to calculate these moments.

For example, we can get the average over the norm of the c-number mode α by a simple average over trajectories of that quantity, and actually then calculate

$$\langle \alpha^* \alpha \rangle = \langle (a^\dagger a + a a^\dagger)/2 \rangle = \langle a^\dagger a \rangle + 1/2.$$

Thus, if we are interested in the occupation number expectation value, we can correct the c-number average as

$$\langle n \rangle = \langle \alpha^* \alpha \rangle - 1/2. \quad (4.29)$$

Similarly, we can calculate

$$\langle (\alpha^* \alpha)^2 \rangle = \langle a^\dagger a^\dagger a a + a^\dagger a a^\dagger a + a^\dagger a a a^\dagger + a a^\dagger a^\dagger a + a a^\dagger a a^\dagger + a a a^\dagger a^\dagger \rangle / 6$$

($4! = 24$ permutations of four different letters $abcd$. We assign a, b to a and c, d to $a^\dagger$. For one $abcd$ permutation, there will be three more that give the same result in terms of $a, a^\dagger$, one with $a \rightarrow b$, one with $c \rightarrow d$ and one with both. Or: We average over all six different orderings none of which is preferred over another.) After trivial algebra, this is seen to be equal to $(6a^\dagger a^\dagger a a + 12a^\dagger a + 3)/6$. Thus,

$$\langle a^\dagger a^\dagger a a \rangle = \langle (\alpha^* \alpha)^2 \rangle - 2 \langle a^\dagger a \rangle - 0.5. \quad (4.30)$$

In the same straightforward way even higher moments of the operators can be expressed in terms of their lower moments.

From the above it is clear that a direct way to get any quantum mechanical expectation value is to obtain the Weyl symbol of the operators and average these. It is also clear that this

can easily be achieved by rewriting the operator as a sum of symmetrically ordered terms, and adding the trivial Weyl symbols of the individual terms. Such a reordering is called Weyl ordering. It is to be distinguished from a symmetrization operation, since the symmetrized version of an operator is typically a *different* operator, while Weyl ordering means expressing the *original* operator as its symmetrization plus corrections.

There is an even easier way to obtain the Weyl symbol, which works by using the coherent state right-acting Bopp representation [Polkovnikov, 2013] of the ladder operators given by

$$a \rightarrow \alpha + \frac{1}{2}\partial_{\alpha^*} \quad (4.31)$$

$$a^\dagger \rightarrow \alpha^* - \frac{1}{2}\partial_{\alpha}. \quad (4.32)$$

This representation is easily checked to obey the canonical commutation relation $[a, a^\dagger] \rightarrow [\alpha + \frac{1}{2}\partial_{\alpha^*}, \alpha^* - \frac{1}{2}\partial_{\alpha}] = 1$. The Weyl symbol of $O(a, a^\dagger)$ is then simply given by

$$O_W(\alpha, \alpha^*) = O\left(\alpha + \frac{1}{2}\partial_{\alpha^*}, \alpha^* - \frac{1}{2}\partial_{\alpha}\right). \quad (4.33)$$

This can straightforwardly be proved for normal ordered operators from definition (4.3) and extends to arbitrary orderings by means of expressing these operators in normal order, using the result for normal order, and reordering the result back after employing the Bopp representation. Since the commutators are the same as in the standard abstract operator case, the Bopp representation so obtained is equivalent to the Bopp representation employed

directly to the original operator. To prove the result for normal order, we have

$$(\alpha^* - \frac{1}{2}\partial_\alpha)^m \alpha^n \quad (4.34)$$

$$= \sum_i \binom{m}{i} (\alpha^*)^{m-1} \left(-\frac{\partial_\alpha}{2}\right)^i \alpha^n \quad (4.35)$$

$$= \sum_i \binom{m}{i} \binom{n}{i} i! \left(-\frac{1}{2}\right)^i (\alpha^*)^{m-1} \alpha^{n-i} \quad (4.36)$$

$$= \frac{1}{2} \sum_i (\alpha^*)^{m-1} \alpha^{n-i} \binom{m}{i} \binom{n}{i} \left(\frac{1}{2}\right)^i \left[\partial_x^i 2x^{-1}\right] \Big|_{x=1} \quad (4.37)$$

$$= \frac{1}{2} \sum_i (\alpha^*)^{m-1} \alpha^{n-i} \binom{m}{i} \binom{n}{i} \left(\frac{1}{2}\right)^i \left[\partial_x^i \int d^2\beta e^{-x|\beta|^2/2}\right] \Big|_{x=1} \quad (4.38)$$

$$= \frac{1}{2} \sum_i (\alpha^*)^{m-1} \alpha^{n-i} \binom{m}{i} \binom{n}{i} \int d^2\beta \left(-\frac{|\beta|^2}{4}\right)^i \left[e^{-x|\beta|^2/2}\right] \Big|_{x=1} \quad (4.39)$$

$$= \frac{1}{2} \sum_i (\alpha^*)^{m-1} \alpha^{n-i} \binom{m}{i} \binom{n}{i} \int d^2\beta \left(-\frac{\beta^*}{2}\right)^i \left(-\frac{\beta}{2}\right)^i \left[e^{-|\beta|^2/2}\right] \quad (4.40)$$

$$= \frac{1}{2} \sum_{i,j} (\alpha^*)^{m-1} \alpha^{n-j} \binom{m}{i} \binom{n}{j} \int d^2\beta \left(-\frac{\beta^*}{2}\right)^i \left(\frac{\beta}{2}\right)^j e^{-|\beta|^2/2} \quad (4.41)$$

$$= \frac{1}{2} \int d^2\beta \left(\alpha^* - \frac{\beta^*}{2}\right)^m \left(\alpha + \frac{\beta}{2}\right)^n e^{-|\beta|^2/2} \quad (4.42)$$

$$= \left((a^\dagger)^m a^n\right)_W \quad (4.43)$$

As an example of this machinery, we can immediately find

$$(a^\dagger a^\dagger a a)_W = (\alpha^* - \frac{1}{2}\partial_\alpha)^2 \alpha^2 = (\alpha^* \alpha)^2 - 2\alpha^* \alpha + 0.5 \quad (4.44)$$

which (after taking the expectation values) agrees with the previous result (4.30) in view of (4.29). Alternatively, formula (4.36) explicitly gives the same result.

4.2.2. Non-equilibrium Path Integral

We employ the Heisenberg picture. Given an initial state ρ (which does not need to be an equilibrium state), we are interested in the expectation values $\langle O \rangle(t)$ of operators O at a later time t in the general case of a time-dependent Hamiltonian,

$$\langle O \rangle(t) = \text{Tr}(\rho O(t)). \quad (4.45)$$

This involves the a priori unknown time-evolution operator $U = T e^{-i \int_0^t dt' H(t')}$ ($\hbar = 1$, and note that T is the time ordering symbol instead of the temperature; the meaning of T is clear from the context). Progress can be made by inserting resolutions of identity into coherent states at different times. The notation we are using is

$$a(t) |\beta(t), t\rangle = \beta(t) |\beta(t), t\rangle, \quad (4.46)$$

that is, the second argument t of the coherent state explicitly indicates that the state is a coherent state at time t . If this t was increased, it would make the state rotate with the inverse evolution operator (just like any other Heisenberg picture operator's eigenstate). The symbol $\beta(t)$ may be fixed when doing that and is not to be understood as a function of time at the moment. It simply stands as a symbol for a particular complex number, but will become a “function” of time, a *path*, below.

We may insert into $Tr(\rho O(t))$ the following resolutions of identity between ρ and $O(t)$:

$$|\alpha(0), 0\rangle \langle \alpha(0), 0| \times |\alpha(\delta t), \delta t\rangle \langle \alpha(\delta t), \delta t| \times \dots \times |\alpha(t), t\rangle \langle \alpha(t), t|, \quad (4.47)$$

including the corresponding integrations $\int d^2\alpha(0) \int d^2\alpha(\delta t) \dots \int d^2\alpha(t)$. Obviously, δt should be chosen an integer fraction of the total time t and will go to zero later. Similarly, we may insert

$$|\beta(t), t\rangle \langle \beta(t), t| \times |\beta(t - \delta t), t - \delta t\rangle \langle \beta(t - \delta t), t - \delta t| \times \dots \times |\beta(0), 0\rangle \langle \beta(0), 0| \quad (4.48)$$

to the right of $O(t)$ with the integrations $\int d^2\beta(0) \int d^2\beta(\delta t) \dots \int d^2\beta(t)$. Evaluating the trace in any orthonormal basis, we are then left with

$$\begin{aligned} & \langle \beta(0), 0 | \rho | \alpha(0), 0 \rangle \langle \alpha(t), t | O(t) | \beta(t), t \rangle \langle \alpha(0), 0 | \alpha(\delta t), \delta t \rangle \times \dots \\ & \times \langle \alpha(t - \delta t), t - \delta t | \alpha(t), \alpha(t) \rangle \langle \beta(t), t | \beta(t - \delta t), t - \delta t \rangle \times \dots \times \langle \beta(\delta t), \delta t | \beta(0), 0 \rangle \end{aligned} \quad (4.49)$$

and the integrations over all $\alpha(0), \dots, \alpha(t), \beta(0), \dots, \beta(t)$.

Considering the scalar product $\langle \alpha(0), 0 | \alpha(\delta t), \delta t \rangle$, we write, making the dependence of the Hamiltonian on the ladder operators explicit,

$$|\alpha(\delta t), \delta t\rangle = T e^{i \int_0^{\delta t} dt' H(a, a^\dagger, t')} |\alpha(\delta t), 0\rangle, \quad (4.50)$$

or, for small enough δt , simply $e^{iH(a, a^\dagger, 0)\delta t} |\alpha(\delta t), 0\rangle$. Suppressing the time indices for a moment, we are thus dealing with terms of the form $\langle \alpha | e^{\pm iH(a, a^\dagger)\delta t} | \alpha' \rangle$. One way to proceed is to expand to first order in δt and put the Hamiltonian into normal order. However, it is more general to assume that the exponential is given in a symmetrized form even to second order. If the Hamiltonian is provided in Weyl-ordered form, it is then palindromic. The square of a palindromic expression is still palindromic. We thus assume that the Hamiltonian has been Weyl-ordered, $H \rightarrow H_W$, and that we then have to deal with a sum of symmetrized terms of the form $\langle \alpha | ((a^\dagger)^r a^s)_S | \alpha' \rangle$ where the subscript S stands for *symmetrized*. We now show that – just as for normal order – this is equal to $(\alpha^*)^r (\alpha')^s \langle \alpha | \alpha' \rangle$. Symmetrized operators with canonical commutators may be written as

$$((a^\dagger)^r a^s)_S = \frac{1}{2^s} \sum_{l=0}^s \binom{s}{l} a^{s-l} (a^\dagger)^r a^l. \quad (4.51)$$

This surprising formula is inspired by a formula in [Bastianelli and Van Nieuwenhuizen, 2006], where it is given for p, q -operators and proven for the case $r = 1$. It says that one of the operator powers (here $(a^\dagger)^r$) may be kept together, and the resulting expression is equal (for canonical commutation relations) to the permutation-symmetrized expression. Inserting a resolution of identity $1 = \int d^2\gamma |\gamma\rangle \langle \gamma|$, we find

$$\langle \alpha | ((a^\dagger)^r a^s)_S | \alpha' \rangle = \int d^2\gamma \frac{1}{2^s} \sum_{l=0}^s \binom{s}{l} \langle \alpha | \gamma \rangle \gamma^{s-l} (\gamma^*)^r \langle \gamma | \alpha' \rangle (\alpha')^l. \quad (4.52)$$

This expression is evaluated by realizing that $\langle \alpha | \gamma \rangle \langle \gamma | \alpha' \rangle e^{|\alpha|^2/2 + |\alpha'|^2/2} = e^{\gamma^* \alpha' + \alpha^* \gamma - |\gamma|^2}$ and

that the moments of γ and γ^* can thus be obtained by partial derivatives as

$$\langle \alpha | ((a^\dagger)^r a^s)_S | \alpha' \rangle \quad (4.53)$$

$$= \int d^2\gamma \frac{1}{2^s} \sum_{l=0}^s \binom{s}{l} e^{-|\alpha|^2/2 - |\alpha'|^2/2} (\alpha')^l \gamma^{s-l} (\gamma^*)^r \langle \alpha | \gamma \rangle \langle \gamma | \alpha' \rangle e^{|\alpha|^2/2 + |\alpha'|^2/2} \quad (4.54)$$

$$= \int d^2\gamma \frac{1}{2^s} \sum_{l=0}^s \binom{s}{l} e^{-|\alpha|^2/2 - |\alpha'|^2/2} (\alpha')^l \frac{\partial^{s-l}}{\partial^{s-l} \alpha^*} \frac{\partial^r}{\partial^r \alpha'} \langle \alpha | \gamma \rangle \langle \gamma | \alpha' \rangle e^{|\alpha|^2/2 + |\alpha'|^2/2} \quad (4.55)$$

$$= \frac{1}{2^s} \sum_{l=0}^s \binom{s}{l} e^{-|\alpha|^2/2 - |\alpha'|^2/2} (\alpha')^l \frac{\partial^{s-l}}{\partial^{s-l} \alpha^*} \frac{\partial^r}{\partial^r \alpha'} \langle \alpha | \alpha' \rangle e^{|\alpha|^2/2 + |\alpha'|^2/2} \quad (4.56)$$

$$= \frac{1}{2^s} \sum_{l=0}^s \binom{s}{l} e^{-|\alpha|^2/2 - |\alpha'|^2/2} (\alpha')^l \frac{\partial^{s-l}}{\partial^{s-l} \alpha^*} \frac{\partial^r}{\partial^r \alpha'} e^{\alpha^* \alpha'} \quad (4.57)$$

$$= \frac{1}{2^s} \sum_{l=0}^s \binom{s}{l} e^{-|\alpha|^2/2 - |\alpha'|^2/2} (\alpha')^l (\alpha')^{s-l} (\alpha^*)^r e^{\alpha^* \alpha'} \quad (4.58)$$

$$= (\alpha')^s (\alpha^*)^r \langle \alpha | \alpha' \rangle, \quad (4.59)$$

where we have avoided carrying out an explicit Gaussian integration by removing the resolution of identity again once the powers of γ and γ^* disappeared. Hence, we have found – partly heuristically – an approximation to the coherent state matrix elements as

$$\langle \alpha(0), 0 | \alpha(\delta t), \delta t \rangle = \langle \alpha(0), 0 | T e^{i \int_0^{\delta t} dt' H(a, a^\dagger, t')} | \alpha(\delta t), 0 \rangle \quad (4.60)$$

$$\approx \langle \alpha(0), 0 | e^{i \delta t H(a, a^\dagger, 0)} | \alpha(\delta t), 0 \rangle \quad (4.61)$$

$$\approx e^{i \delta t H_W(\alpha(\delta t), \alpha^*(0), 0)} \langle \alpha(0), 0 | \alpha(\delta t), 0 \rangle \quad (4.62)$$

$$= e^{i \delta t H_W(\alpha(\delta t), \alpha^*(0), 0)} e^{\alpha^*(0) \alpha(\delta t) - |\alpha(0)|^2/2 - |\alpha(\delta t)|^2/2}. \quad (4.63)$$

Note that for all intermediate time states at $\tau \neq 0, \neq t$ a complex number $\alpha(\tau)$ or $\beta(\tau)$ appears twice at the scalar product to both the left and the right of the inserted resolution of identity, and we get a term $-|\alpha(\tau)|^2$ or $-|\beta(\tau)|^2$ in the exponent. At the boundary, we get only half that value. In total, for β , we have the following terms in the exponent

$$e^{-|\beta(t)|^2/2 - |\beta(0)|^2/2} e^{\beta^*(t) \beta(t - \delta t) - |\beta(t - \delta t)|^2 + \beta^*(t - \delta t) \beta(t - 2\delta t) - |\beta(t - 2\delta t)|^2 + \dots + \beta^*(2\delta t) \beta(\delta t) - |\beta(\delta t)|^2 + \beta^*(\delta t) \beta(0)}, \quad (4.64)$$

which can be rewritten by adding and subtracting $|\beta(t)|^2$ as

$$e^{|\beta(t)|^2/2 - |\beta(0)|^2/2} e^{-\beta^*(t) (\beta(t) - \beta(t - \delta t)) - \dots - \beta^*(\delta t) (\beta(\delta t) - \beta(0))}. \quad (4.65)$$

There is an equivalent rewriting of form (4.65) with the signs in both exponents reversed, and non-conjugated β s at the earlier time multiplying differences of conjugated ones at two different times, like $+\beta(0)(\beta^*(\delta t) - \beta^*(0))$. Similarly, we collect for the α the terms

$$e^{|\alpha(0)|^2/2 - |\alpha(t)|^2/2} e^{\alpha^*(0)(\alpha(\delta t) - \alpha(0)) + \dots + \alpha^*(t - \delta t)(\alpha(t) - \alpha(t - \delta t))} \quad (4.66)$$

$$\approx e^{|\alpha(0)|^2/2 - |\alpha(t)|^2/2} e^{\int_0^t dt' \alpha^*(t') \frac{d}{dt'} \alpha(t')}. \quad (4.67)$$

Here we have written what would be an approximation for small δt assuming that the $\alpha(\tau)$ form a function which has the required properties for such an expression to be well-defined. While not rigorous, we may use this notation as a short-hand. For β we have

$$e^{|\beta(t)|^2/2 - |\beta(0)|^2/2} e^{-\int_0^t dt' \beta^*(t') \frac{d}{dt'} \beta(t')}. \quad (4.68)$$

The two equivalent rewritings in each case correspond to partial integration in the integral form.

In the limit $\delta t \rightarrow 0$, the products of all the exponentiated Hamiltonians evaluated at intermediate times and intermediate values of the complex functions $\alpha(\tau), \beta(\tau)$ (where to first order we can neglect the fact that one variable is coming in at a slightly different time) yields

$$e^{i \int_0^t dt' H_W(\alpha(t'), \alpha(t'), t')} \quad \text{and} \quad e^{-i \int_0^t dt' H_W(\beta(t'), \beta(t'), t')}. \quad (4.69)$$

Combining the integrations in a functional measure $D^2\alpha D^2\beta$, we find, all together,

$$\begin{aligned} \langle O \rangle(t) &= \int D^2\alpha D^2\beta \langle \beta(0), 0 | \rho | \alpha(0), 0 \rangle \langle \alpha(t, t) | O(t) | \beta(t), t \rangle \\ &e^{|\beta(t)|^2/2 - |\beta(0)|^2/2 + |\alpha(0)|^2/2 - |\alpha(t)|^2/2} \\ &e^{i \int_0^t dt' H_W(\alpha(t'), \alpha(t'), t') - i \int_0^t dt' H_W(\beta(t'), \beta(t'), t')} e^{\int_0^t dt' \alpha^*(t') \frac{d}{dt'} \alpha(t') - \int_0^t dt' \beta^*(t') \frac{d}{dt'} \beta(t')} \end{aligned} \quad (4.70)$$

Change of variables Using partial integration, we may easily verify that

$$\int_0^t dt' \left(\alpha^*(t') \frac{d}{dt'} \alpha(t') - \beta^*(t') \frac{d}{dt'} \beta(t') \right) \quad (4.71)$$

$$+ |\beta(t)|^2/2 - |\beta(0)|^2/2 + |\alpha(0)|^2/2 - |\alpha(t)|^2/2 \quad (4.72)$$

$$\begin{aligned} &= \int_0^t dt' \left((\alpha^*(t') - \beta^*(t')) \frac{d}{dt'} \frac{\alpha(t') + \beta(t')}{2} - (\alpha(t') - \beta(t')) \frac{d}{dt'} \frac{\alpha^*(t') + \beta^*(t')}{2} \right) \\ &+ ((\alpha\beta^*)(t) - (\beta\alpha^*)(t))/2 - ((\alpha\beta^*)(0) - (\beta\alpha^*)(0))/2. \end{aligned} \quad (4.73)$$

It is convenient to introduce the variables

$$\begin{aligned}\phi &= (\alpha + \beta)/2 & \alpha &= \phi + \psi/2 \\ \psi &= \alpha - \beta & \beta &= \phi - \psi/2,\end{aligned}\tag{4.74}$$

with which we can write equation (4.73) (since, as a short calculation shows, $\alpha\beta^* - \beta\alpha^* = \psi\phi^* - \phi\psi^*$) as

$$\begin{aligned}& \int_0^t dt' \left(\psi^*(t') \frac{d}{dt'} \phi(t') - \psi(t') \frac{d}{dt'} \phi^*(t') \right) \\ & + ((\psi\phi^*)(t) - (\phi\psi^*)(t))/2 - ((\psi\phi^*)(0) - (\phi\psi^*)(0))/2.\end{aligned}\tag{4.75}$$

With these new variables, we then have

$$\begin{aligned}\langle O \rangle(t) &= \int D^2\phi D^2\psi \langle \phi(0) - \psi(0)/2, 0 | \rho | \phi(0) + \psi(0)/2, 0 \rangle \\ &\times \langle \phi(t) + \psi(t)/2, t | O | \phi(t) - \psi(t)/2, t \rangle \\ &\times e^{((\psi\phi^*)(t) - (\phi\psi^*)(t))/2 - ((\psi\phi^*)(0) - (\phi\psi^*)(0))/2} \\ &\times e^{\int_0^t dt' \left(\psi^*(t') \frac{d}{dt'} \phi(t') - \psi(t') \frac{d}{dt'} \phi^*(t') \right)} \\ &\times e^{\int_0^t dt' (iH_W(\phi(t') + \psi(t')/2, \phi^*(t') + \psi^*(t')/2, t') - iH_W(\phi(t') - \psi(t')/2, \phi^*(t') - \psi^*(t')/2, t'))},\end{aligned}\tag{4.76}$$

since the change of variable has unit determinant for each pair in $\mathbf{C}^2$, as another short calculation shows.

Exact expression without integral calculus One may, after hard work, arrive at the following *discretized* rewriting for the exponent, which is equivalent to our starting point (4.65) and (4.66), combining as in (4.77), and which cannot be deduced from the integral form (4.75)

and indeed differs from it for paths that are not well behaved enough,

$$\sum_{n=0}^{N-1} [\alpha_n^*(\alpha_{n+1} - \alpha_n) + \beta_n(\beta_{n+1}^* - \beta_n^*)] + |\alpha_0|^2/2 - |\alpha_N|^2/2 + |\beta_0|^2/2 - |\beta_N|^2/2 \quad (4.77)$$

$$\begin{aligned} = & \sum_{n=0}^{N-1} \left[\frac{\psi_{n+1}^* + \psi_n^*}{2} (\phi_{n+1} - \phi_n) - \frac{\psi_{n+1} + \psi_n}{2} (\phi_{n+1}^* - \phi_n^*) \right. \\ & \left. - 2|\phi_n|^2 - |\psi_n|^2/2 + 2 \operatorname{Re}\{\phi_{n+1}^* \phi_n + \psi_{n+1}^* \psi_n/4\} \right] \\ & + |\phi_0|^2 + |\psi_0|^2/4 - |\phi_N|^2 - |\psi_N|^2/4 \\ & + (\phi_0 \psi_0^* - \psi_0 \phi_0^*)/2 - (\phi_N \psi_N^* - \psi_N \phi_N^*)/2. \end{aligned} \quad (4.78)$$

Here, a subscript n stands for $\tau = n\delta t$. Note that the first line of the result is imaginary. The second part in the sum, in the third line, is real and vanishes for smooth paths: it contains terms $-|\alpha_n|^2 - |\beta_n|^2 + \operatorname{Re}\{\alpha_{n+1}^* \alpha_n + \beta_{n+1}^* \beta_n\}$ and is equal to the sum over $-|\alpha_{n+1} - \alpha_n|^2/2 - |\beta_{n+1} - \beta_n|^2/2$ from $n = 0$ to $n = N - 1$ up to boundary terms. When α and β are continuous and can be Taylor expanded to first order, this is a sum of terms quadratic in the differences of neighbors and $\propto N^{-2}$, and the sum of $\propto N$ such terms vanishes in the limit $N \rightarrow \infty$. The remaining terms are boundary terms.

Wigner Transforms The functionals $\int_0^t dt' \left(\psi^*(t') \frac{d}{dt'} \phi(t') - \psi(t') \frac{d}{dt'} \phi^*(t') \right)$ as well as $\pm \int_0^t dt' H'_W(\phi(t'), \psi(t'), dt')$ do not depend on the (finite) values of the argument function ψ at any countable set of points in the continuum limit, including the values of $\psi(0)$ and $\psi(t)$ at the boundary. Indeed, no time derivative of ψ appears under the integral, meaning that at every time slice t' , $\psi(t')$ is fully independent of its neighboring values.³ The assumption we must make for this argument is, however, that the time derivative of $\phi(t')$ is bounded, i.e. $\phi(t')$ is continuous. This can be achieved by discretizing the integrals over the $\phi(t')$'s at each time slice t' followed by a resummation, which can be made explicit by changing the functional integration measure to one over mode amplitudes. Such changes of integration variables can be calculated rigorously [Brown, 1994]. We assume from now on that the integration over $\phi(t')$ is over continuous paths, and we therefore may carry out the integration

³A partial integration to introduce time derivatives of ψ instead of ϕ would also generate further boundary terms cancelling the apparently introduced dependence on the boundary values.

over $\psi(0)$ and $\psi(t)$ restricted to

$$\begin{aligned} & \int d^2\psi(0) \langle \phi(0) - \psi(0)/2, 0 | \rho | \phi(0) + \psi(0)/2, 0 \rangle e^{-((\psi\phi^*)(0) - (\phi\psi^*)(0))/2} \\ & = 2W(\phi(0), \phi^*(0)) \end{aligned} \quad (4.79)$$

$$\begin{aligned} & \int d^2\psi(t) \langle \phi(t) + \psi(t)/2, t | O | \phi(t) - \psi(t)/2, t \rangle e^{((\psi\phi^*)(t) - (\phi\psi^*)(t))/2} \\ & = 2O_W(\phi(t), \phi(t)^*). \end{aligned} \quad (4.80)$$

Note that for $\psi(t')$, unlike for $\phi(t')$, we keep the discontinuous paths, integrating first at fixed time for the boundaries as well as the inner points $0 < t' < t$.

An apparent confusion may arise in view of approximating the value of the path integral by the method of stationary phase, which may seem to indicate a dependence on the boundary conditions of ψ . To identify the interfering paths that contribute most to the path integral around the vanishing first variation seems to set a continuity condition and boundary conditions on $\psi(t')$ (this will be discussed explicitly below): While the values of $\psi(t')$ at different times are not directly coupled to each other, the function $\phi(t')$ does have this property. Thus, a variation of e.g. $\phi(\delta t)$ of an adjacent field value, as it occurs in a stationary phase approximation below, couples to $d\phi(t')/dt'(0)$ and then also to $\psi(0)$. We argue that again for assuming *continuous variations* of $\delta\phi(t')$, and in the continuum limit, this does not pose a problem.⁴ Thus, we *will* soon deal with continuous “stationary” functions $\psi_0(t')$

⁴For clarity, consider the example of a discretized action of the form $\int_0^T (p(t)\dot{q}(t) - p^2/2mV(q(t)))dt$ with p playing the role of ψ and q the role of ϕ . It is evident that even though p could be changed at any point including $t = 0$ without changing the *value* of the functional for continuous $q(t)$, for the action to be *stationary* with respect to $q(\delta t) \equiv q_1 \rightarrow q_1 + \delta q_1$ for finite δq_1 , we do need the discretized variation to vanish

$$\begin{aligned} 0 &= p_0(q_1 + \delta q_1 - q_0) + p_1(q_2 - q_1 - \delta q_1) + \dots - V(q_0)\delta t - V(q_1 + \delta q_1)\delta t - \dots \\ & \quad - p_0(q_1 - q_0) + p_1(q_2 - q_1) + \dots - V(q_0)\delta t - V(q_1)\delta t - \dots \\ &= [(p_0 - p_1) - V'(q_1)\delta t]\delta q_1, \end{aligned}$$

which clearly involves a coupling of p_0 and p_1 , in fact forcing $p(t)$ to be differentiable. Indeed the Euler-Lagrange equations would also imply this. However, these equations only follow from the variation of the integral action under certain mathematical assumptions related to integration theory and variational calculus. If the continuum limit is such that $\delta q_1 \rightarrow 0$ to restore continuity of $\delta q(t)$, which vanishes at the

with well-defined boundary values at $t' = 0$, $t' = t$, but they will arise only for calculational purposes to obtain an approximation to the full path integral, and its boundary values do not need to be identified with the arbitrary values that have just been integrated out.

We are now able to write (with an updated definition of the measure $D^2\psi^o$ that excludes integration over $\psi(0)$ and $\psi(t)$)

$$\begin{aligned} \langle O \rangle(t) = & 4 \int D^2\phi D^2\psi^o W(\phi(0), \phi^*(0)) O_W(\phi(t), \phi^*(t)) \\ & \times e^{\int_0^t dt' (\psi^*(t') \frac{d}{dt'} \phi(t') - \psi(t') \frac{d}{dt'} \phi^*(t'))} \\ & \times e^{\int_0^t dt' (iH_W(\phi(t') + \psi(t')/2, \phi^*(t') + \psi^*(t')/2, t') - iH_W(\phi(t') - \psi(t')/2, \phi^*(t') - \psi^*(t')/2, t'))}. \end{aligned} \quad (4.81)$$

To make progress, it is useful to assume that $\psi(t)$ is a small quantity. Paraphrasing [Polkovnikov, 2013], the difference of the forward and backward propagating quantities α, β , should be equal in the classical limit, when only one deterministic path is realized. Thus, $\psi(t) \neq 0$ can be thought of the quantum fluctuations, whereas $\phi(t)$ plays the role of a classical field.

Stationary Phase Approximation Mathematically speaking, we are simply interested in a stationary phase approximation finding paths that interfere constructively. Since we have multiple fields, we can in principle vary any, and obtain the corresponding equations of motion. On shell the action (the integral in the exponent of the path integral) is then stationary with respect to the variation of one variable, meaning that paths interfere constructively for arbitrary small fluctuations of that variable. The equations, however, typically contain the other variables as well (or even exclusively contain the other variables). Indeed, the variation with respect to the quantum field ψ^* gives the equation for ϕ_0

$$\partial_t \phi_0 + \frac{i}{2} \frac{\partial H_+(\phi_0, \psi)}{\partial \phi_0^*} + \frac{i}{2} \frac{\partial H_-(\phi_0, \psi)}{\partial \phi_0^*} = 0, \quad (4.82)$$

boundary, $p(t)$ is allowed to jump at the boundary. Similarly, it may be modified at a countable set of points throughout the interval, which also gives only a sum of terms proportional to $(q_n - q_{n-1})$ which vanish in the same limit (jumps without returning inside the interval are however not allowed). Thus, just as in the case for the argument of the functional value being independent of modifications at the boundary in the continuum limit for continuous functions $\phi(t)$, even for the stationarity condition we can establish such an independence for a strongly related assumption of continuous variations $\delta\phi(t)$.

with $H_{\pm}(\phi_0, \psi) := H_W(\phi_0 \pm \psi/2, \phi_0^* \pm \psi/2)$. Here we have added a 0 subscript to indicate that the solution describes the semi-classical limit.

Note that if ψ is very small (allowing to expand $H_{\pm}$ to zeroth order in ψ in (4.82), i.e. setting $\psi = 0$, or expanding to first order in the action), we recover the GPE for ϕ_0 .

Unlike for variations of ψ , for variations $\delta\phi$ of ϕ around the solution ϕ_0 of (4.82) paths may not yet interfere constructively. The corresponding equations for this variation can, however, simultaneously be satisfied, imposing conditions on ψ_0 via

$$\partial_t \psi_0^* - i \frac{\partial H_+(\phi_0, \psi_0)}{\partial \phi_0} + i \frac{\partial H_-(\phi_0, \psi_0)}{\partial \phi_0} = 0. \quad (4.83)$$

For $\psi_0 = 0$, $H_+(\phi_0, \psi_0) = H_-(\phi_0, \psi_0)$, and hence we see that $\psi_0 = 0$ is a solution of the previous equation at all times if it initially was zero. In this case, the GPE for ϕ_0 is exactly obtained from (4.82) and we have found a stationary point of the full system with fluctuations in both ψ and ϕ interfering constructively⁵

In general, however, the path integral includes the integrations over $\phi(0)$ and $\phi(t)$, which can be made explicit as

$$\begin{aligned} \langle O \rangle(t) = 4 \int d^2\phi(0) d^2\phi(t) \left\{ \int D^2\phi^o D^2\psi^o W(\phi(0), \phi^*(0)) O_W(\phi(t), \phi^*(t)) \right. \\ \left. \times e^{\int_0^t dt' (\psi^*(t') \frac{d}{dt'} \phi(t') - \psi(t') \frac{d}{dt'} \phi^*(t') + iH_+(\phi, \psi, t') - iH_-(\phi, \psi, t'))} \right\}, \end{aligned} \quad (4.84)$$

and which poses sufficient boundary conditions for the first-order system consisting of the two complex equations (4.82, 4.83). This means that in a stationary phase approximation of the path integral in the braces of (4.84), for any boundary values set by the integration over the boundary values for ϕ , the classical equations of motion determine the boundary values of ψ_0 . If $\phi(t) = \phi_0(t)$ is equal to the value of the GPE evolution of $\phi(0) = \phi_0(0)$, ψ_0 is determined to vanish. If it is close to equal, ψ_0 is expected to be small throughout the evolution.

To derive TWA, we assume that it indeed is small; however, it should be noted that the stationary phase approximation goes beyond this assumption by including stationary paths

⁵Due to the Weyl ordering, an equation that is physically equivalent to the GPE evolution is obtained in the case of a homogeneous BEC. See [Polkovnikov, 2010] for details.

for large deviations. It is expected that further analysis would show that for large $|\phi| \gg 1$ the additional assumption is well justified. Studying this further would be a very interesting direction of research.

Deriving TWA We already know that we obtain the GPE for ϕ_0 for small ψ , but we have not yet calculated the value of the path integral, that is of the expectation value of an operator, itself. Given our assumptions, we may carry out a Taylor expansion of the functional to second order in ψ . The quadratic order vanishes, and the linear order is going to produce delta functions. After the expansion, the action S reads

$$S = \int_0^t dt' \left(\psi^*(t') \frac{d}{dt'} \phi(t') - \psi(t') \frac{d}{dt'} \phi^*(t') + i \frac{\partial H_W(\phi(t), \phi^*(t))}{\partial \phi} \psi(t') + i \frac{\partial H_W(\phi(t), \phi^*(t))}{\partial \phi^*} \psi^*(t') \right) \quad (4.85)$$

$$= \int_0^t dt' 2i \operatorname{Im} \left(\left\{ \frac{d}{dt'} \phi(t') + i \frac{\partial H_W(\phi(t), \phi^*(t))}{\partial \phi^*} \right\} \psi^*(t') \right) \quad (4.86)$$

$$= \int_0^t dt' \left\{ i \operatorname{Im} \left(\frac{d}{dt'} \phi(t') + i \frac{\partial H_W(\phi(t), \phi^*(t))}{\partial \phi^*} \right) 2 \operatorname{Re}(\psi^*(t')) \right. \quad (4.87)$$

$$\left. + i \operatorname{Re} \left(\frac{d}{dt'} \phi(t') + i \frac{\partial H_W(\phi(t), \phi^*(t))}{\partial \phi^*} \right) 2 \operatorname{Im}(\psi^*(t')) \right\} \quad (4.88)$$

After writing the integral in discretized form again, the integration $\int d^2 \phi(\tau) = (4\pi)^{-1} \int d2 \operatorname{Re}(\phi(\tau)) d2 \operatorname{Im}(\phi(\tau))$ at an intermediate time slice τ over the exponentiated action e^S simply produces

$$\pi \delta \left(\operatorname{Re} \left(\phi(\tau + \delta t) - \phi(\tau) + i dt' \frac{\partial H_W(\phi(\tau), \phi^*(\tau))}{\partial \phi^*} \right) \right) \quad (4.89)$$

$$\times \delta \left(\operatorname{Im} \left(\phi(\tau + \delta t) - \phi(\tau) + i dt' \frac{\partial H_W(\phi(\tau), \phi^*(\tau))}{\partial \phi^*} \right) \right) \quad (4.90)$$

assuming a forward-differencing discretization of the derivative.

The remaining factor of π cancels with the $1/\pi$ in the definition of the measure for $d^2 \phi(\tau + \delta t)$, which can be integrated out next. We may specialize to $\tau = t - \delta t$, such that now the integration is over $\phi(t)$, one time step later than the last delta function produced by integration over $\psi(t - \delta t)$. This sets $\phi(t)$ to be equal to $\phi(t - \delta t)$ evolved in time according to the GPE by one timestep. This procedure can be continued as now the only remaining dependence on $\phi(t - \delta t)$ is linear in the second to last delta functions. The iteration stops with the

integration over $\phi(2\delta t)$, which comes out as GPE-evolved from $\phi(\delta t)$ by the delta functions created when integrating over $\psi(\delta t)$. All factors of π have now been cancelled.

There are two details in this calculation that do not come out as expected. First, we would have liked to connect to $\phi(0)$ instead of $\phi(\delta t)$. Second, we have a factor of 4 in (4.84), which should not appear to give the expected result (4.16) for the expectation value in the limit of vanishing evolution time. These problems have not been discussed in the slightly different approaches in the literature, and are partly hidden there in using wrong definitions of the Wigner transformation that cancel the factor of 4. It should be clear that a full derivation with all factors coming out correctly *can only be* given by considering the full, exact discretized form we have given in equation (4.78). It is well known that being cavalier with the notation for path integrals in QFT leads even to infinite constants that are determined by other arguments. Here, it is clear that the 4 should be cancelled. For an exact evaluation, the arguments leading to the Wigner transforms in (4.79, 4.80) and the derivation given in this subsection have to be modified accordingly. The resulting calculations are lengthy and left for future work that can build on result (4.78). This equation is the basis of a more rigorous understanding of the path integral where the limit of $\delta t \rightarrow 0$ is carried out in the very end, which may lead to better understanding of approximations and further new insight.

4.2.3. Observables

Arbitrary Mode Correlations from Classical Field

In the previous section we have shown that the classical field evolution sampled initially from the Wigner function approximates the nonequilibrium path integral. We have considered coherent states of a single, arbitrary mode. In the multi-mode generalization, we could take the coherent states to be eigenstates of the momentum mode annihilation operators and express the Hamiltonian in terms of these to obtain the classical equations of motion. The interaction term leads to a convoluted sum in Fourier space, which is hard to evaluate numerically. In real space, the GPE nonlinearity instead becomes a trivial power.

We thus take the approach to derive TWA for the real-space field. Despite the coupling of

modes due to the kinetic term in the Hamiltonian, the derivation of the the single-mode case of the previous section goes through with trivial changes.

Although deriving TWA from the real-space perspective, we are interested in expectation values of products of momentum operator eigenstate creators/annihilators. The reason is that the phononic excitations that we want to parametrically excite involve momentum modes lying on a shell for a certain wave vector modulus $k = |\mathbf{k}|$ in the homogeneous system. These expectation values are (n-fold) Fourier transforms of the corresponding real-space field operator moments. We argue that these correspond to the c-field moments of the Fourier transformed field from the real-space simulation, namely in such a way that the Weyl mapping can be evaluated in Fourier space directly.

To see this, it is best to Weyl order the momentum operators first. It should be sufficient to consider an example case instead of a completely general proof. We take

$$\langle \hat{n}_k \rangle = (\hat{a}_k^\dagger \hat{a}_k + \hat{a}_k \hat{a}_k^\dagger - 1)/2. \quad (4.91)$$

Now, we may represent the constant term -1 as (in the following expression, $k_1 = k_2$ for this example, but we write the general results)

$$-\delta_{k_1 k_2} = [\hat{a}_{k_1}^\dagger, \hat{a}_{k_2}] \quad (4.92)$$

$$= - \int_V dx_1 \int_V dx_2 e^{-ik_1 x_1 + ik_2 x_2} \delta(x_1 - x_2)/V. \quad (4.93)$$

This allows writing the whole *Weyl ordered* expression as *one* 2-fold Fourier transform after taking out the integration of the sum of terms, since e.g.

$$\hat{a}_{k_1} \hat{a}_{k_2}^\dagger = \int_V dx_1 \int_V dx_2 e^{-ik_1 x_1 + ik_2 x_2} \hat{\Psi}(x_1) \hat{\Psi}^\dagger(x_2). \quad (4.94)$$

The single integrand of this single double integral is then also symmetrically ordered in the real-space field operators. Taking the quantum expectation value inside, the real-space operators can thus simply be replaced by the ensemble average of the c-number field. Now, the Fourier transform may be inserted in the expectation value, and the original commutator terms from the Weyl ordering are reproduced by going from the right to the left in the identity (4.92). Thus, the averages of momentum mode creators/annihilators we wanted to compute correspond to the average of the components of the Fourier transformed field.

Clearly, this way of transforming the c-field first and averaging later depends only on the linearity and canonical (commutator preserving) nature of the Fourier transform and holds for all creators/annihilators for an arbitrary single-particle basis.

Similarly, we can argue that even for the mode-mixing Bogoliubov transformation, we obtain the quasiparticle expectation values by averaging the classically Bogoliubov-transformed field, since this transformation also preserves the property of symmetrical ordering.

Two-mode Variance and Cauchy-Schwarz Inequality

Assuming a perfectly two-mode squeezed thermal state as predicted within Bogoliubov theory, only the cross- and autocorrelations are necessary for evaluating the TMV (2.5). These are, with the rules discussed in Section 4.2.1, easily seen to be given as

$$G_{a,a}^{(2,2)} = \langle (\alpha^* \alpha)^2 - 2\alpha^* \alpha + 0.5 \rangle \quad (4.95)$$

$$G_{a,b}^{(2,2)} = \langle \alpha^* \alpha \beta^* \beta - \alpha^* \alpha + 0.25 \rangle. \quad (4.96)$$

Here, $\beta = \phi_{-k}$ is the Fourier mode for the negative value of $\mathbf{k}$ with respect to $\alpha = \phi_k$ and we have made use of $\langle \alpha^* \alpha \rangle = \langle \beta^* \beta \rangle$. In fact, despite the prediction of this symmetry in the ideal case, even if it is *not* exactly realized for a finite number of trajectories due to the noisy sampling (or in experiment), eventually at the data analysis stage an angular average is carried out over all $\mathbf{k}$ with $|\mathbf{k}|$ within some bin width (which may be chosen to be a fraction of about one percent of the considered full range of momenta, such that for standard grid sizes even in two dimension enough noise reduction is achieved). After this averaging the symmetry is always strictly enforced.

For each saved time step, we calculate a matrix (2D) or tensor (3D) for each $G_{a,a}^{(2,2)}$ as well as $G_{a,b=-a}^{(2,2)}$ of the size of the field, each as averages over the trajectories (here a takes values in the 2D or 3D Fourier space). Only these correlators (and a few other observables) are kept, and the data of the individual trajectories is deleted. The angular average is carried out in the data analysis step in the end, separating these two averaging processes.

Note that the perfect two-mode squeezing is an idealization within Bogoliubov theory. The

two-mode variance can be calculated more accurately beyond that approximation from its definition (2.3), if required.

Mode Entanglement

Within Bogoliubov theory, the TMV and CSI are sufficient to conclusively determine separability of the modes for the two-mode squeezed state, that is, they are sufficient and necessary. General mode entanglement for other Gaussian states or non-Gaussian states can be sufficiently detected by the criterion (2.20). A generally sufficient and necessary criterion for Gaussian states was first derived in [Simon, 2000]. We have implemented this criterion by including the entries of the covariance matrix in the list of observables.

Beyond Gaussianity, entanglement may be hidden in higher moments. In [Shchukin and Vogel, 2005] a hierarchy of criteria necessary and sufficient for detecting a violation of the positive partial transpose (PPT)-criterion of separability [Peres, 1996] has been discovered, which naturally includes higher moments.⁶

One non-trivial criterion (for two-mode squeezed states) of next order that can be derived from this hierarchy is

$$|\langle aabb \rangle| > \langle a^\dagger abb^\dagger \rangle = n_k + G_{a,b}^{(2,2)}. \quad (4.97)$$

Satisfying this criterion is *always* sufficient for entanglement because it implies a violation of the PPT criterion (since the opposite statement is necessary for a PPT state among all the others of the hierarchy), and a separable state must be a PPT state.

Note that because of $U(1)$ symmetry of the theory the left hand side is zero in a BEC unless one sets, as we have done in Section 1.2, the condensate phase to zero and breaks the symmetry. This is the same as developing the theory relative to the condensate phase. Therefore, we should really understand our operators a and b as containing a cancellation

⁶For Gaussian states, the hierarchy can stop at the second moments, which contain all information about the state, and the obtained criterion is not only equivalent to a violation PPT but also to nonseparability itself, i.e. to the aforementioned criterion in [Simon, 2000].

factor for the condensate phase. In the TWA simulations, where the condensate phase is evolving and thus does not remain zero (and may even be chosen randomly in the first place), we thus have to rotate the fourth moment by the condensate phase angle times minus four before averaging the field modes. Similar considerations apply, of course, already to the anomalous real particle density $\langle ab \rangle$, which also has to vanish unless the operators are understood w.r.t. the condensate. Thus, what can be entangled are either the condensate phase counter-rotated momentum modes of the atoms, or the quasiparticles (the condensate phase, if not vanishing, is actually explicitly entering the transformation to quasiparticles for diagonalizing the Hamiltonian), but never the pure momentum modes of the atoms (c.f. Section 4.2.3) including the random phase, since the anomalous density vanishes and the mode CSI can never be satisfied.

While we have successfully proven entanglement using this criterion (4.97), we have not seen cases where it is satisfied while lower moments criteria are not, and it is not clear if other cases exist where the higher order criterion really is more powerful.

Dispersion Relation

Following [Davis et al., 2001], we determine a modified dispersion relation in the presence of sufficiently strong interactions by measuring the phase evolution speed in the Bogoliubov basis. This means that we keep the basis of the normal modes fixed, and assume that (classical) effects on the diagonal representation due to the interaction beyond Bogoliubov theory can be accounted for by modification of the energy levels of these basis functions in the spirit of first-order perturbation theory.

This is expected to only work in the microcanonical, thermalized setting, that is, for time averages after sufficiently long relaxation times. Typically, we average over ca. 100 instances spread out in the later part of the simulation.

Gaussianity

The Gaussianity can be checked by testing factorization of moments of the mode operators. The modes where we expect Gaussianity in the Bogoliubov regime can be quasiparticles or real particles with the condensate phase cancelled as explained above. The actual real-particle operators without this cancellation are not related by a simple two-mode squeezing to the quasiparticles since the squeezing coefficients are now dependent on the particular realization of the ensemble.

We consider moments of at least quartic order, and the absolute value of the difference to its factorization into quadratic moments assuming Gaussianity. We then divide this quantity by the absolute value of the higher moment or alternatively its factorization to obtain a relative error. This gives zero in the perfectly Gaussian case and $\ll 1$ when Gaussianity is almost given. If on the other hand e.g. one expression is by a factor of two larger than the other, corresponding to very strong departure from Gaussianity, it is either 0.5 or 1 depending if the larger quantity is the one that one compares the difference to or not. Such expressions can be averaged for multiple moments.

We select the (normally ordered) real- and quasiparticle intensity autocorrelation as well as the quasiparticle intensity cross-correlations for carrying out this factorization test. We observe that all separate tests show similar behavior, which partly justifies to focus on three of them only.⁷

A more rigorous implementation of a Gaussianity check would calculate and check *all* moments up to some order. However, our method is already sufficient for detecting non-Gaussianity, as we will see.

⁷The real-particle cross-correlations factorize into an expression containing the real-particle anomalous density, which at the point of the implementation of this feature had not been of interest and is not included in the post-processing code.

4.2.4. Comparison of Classical Simulations and TWA

We have seen in Section 4.2.2 that a crucial ingredient of the TWA method is the mapping of operators and their functional representation, with moments of the Wigner function corresponding specifically to symmetrically ordered operator moments. This introduces crucial correction terms for other operators, for example as they appear in correlation measures used to investigate the “quantumness” of the system such as the TMV (described in the first part in Chapter 2 as well as the previous sections).

This mapping is carried out at any point in time when averaging over the trajectories, even long after the initial sampling. On the other hand, TWA produces the correct quantum results only for short enough times. For long times, each trajectory becomes equal to a PGPE simulation, which is known to reach the classical result of equipartition of energy instead of a Bose-Einstein distribution in a microcanonical sense. The average over many such trajectories at a particular time with sampled, noisy initial conditions is similar to a canonical ensemble and would give comparable results. The precise noise statistics for each mode, which is crucial to reproduce Bogoliubov theory exactly at the initial time and which is not equal to the Boltzmann distribution of the canonical ensemble, is expected to wash out after long times and is not important for the correspondence to the microcanonical ensemble. The noise is simply responsible for starting the simulation at different points in the classical phase space for each trajectory.

For short times, when the precise statistics are relevant when sampling the Gaussian Wigner function of the state, there is an additional “quantum” ingredient in the TWA method other than the mapping that disappears after a sufficiently long time. The question is what the relative relevance of these two ingredients is and if they can be distinguished. We investigate this further with the goal to learn about the timescale after which the TWA has converted itself to a classical simulation like PGPE with the mapping from symmetrically ordered to the relevant products of operators as the only remaining “quantum” ingredient.

To this end, we may consider any (quantum) observable, and map it – assuming the validity of the TWA simulation – to ensemble averages of the classical field. For example we may

consider

$$\langle a^\dagger a a^\dagger a \rangle = \langle (a^\dagger a a^\dagger a)_{sym} \rangle - \left(\langle a^\dagger a \rangle + \frac{1}{2} \right) = \langle \alpha^* \alpha^* \alpha \alpha \rangle - \langle \alpha^* \alpha \rangle. \quad (4.98)$$

As a remark, note that within the quantum theory, a Wick factorization holds also for the symmetrically ordered moments, i.e. the moments of the (Gaussian) Wigner function on the right hand side. Thus, we can use the Wick theorem on the moments of α, α^* understanding these as labels for symmetrized operator expressions. This is interesting since it works even though the state is *not* the classical thermal two-mode squeezed state (equipartition) unlike in the first part of the thesis. Using this observation, we can further manipulate the expression still giving the quantum expectation value $\langle a^\dagger a a^\dagger a \rangle$ as

$$\begin{aligned} \langle \alpha^* \alpha^* \alpha \alpha \rangle_{cl} - \langle \alpha^* \alpha \rangle_{cl} &= 2 \langle \alpha^* \alpha \rangle_{cl}^2 + |\langle \alpha^2 \rangle_{cl}|^2 - \langle \alpha^* \alpha \rangle_{cl} \\ &= 2 \langle \alpha^* \alpha \rangle_{cl}^2 - \langle \alpha^* \alpha \rangle_{cl}. \end{aligned} \quad (4.99)$$

(assuming for simplicity that the term $\langle \alpha^2 \rangle$ vanishes despite referring to the phase w.r.t. the condensate, as in the ideally two-mode squeezed case). Using the mapping once more, this is then shown to be equivalent to $2 \langle a^\dagger a \rangle^2 + \langle a^\dagger a \rangle$ with a plus sign. Note that this is indeed consistent with the same result obtained by normal ordering $\langle a^\dagger a a^\dagger a \rangle$ and using the Wick rule on the normally ordered quantum moments (which holds since also the P-distribution is Gaussian). Evaluating either of the expressions in (4.99) with the simulation (“(measured by simulation)”), we can compare this to the prediction for $\langle a^\dagger a a^\dagger a \rangle = 2 \langle a^\dagger a \rangle^2 + \langle a^\dagger a \rangle = 2n_k^2 + n_k$ in the notation of Chapter 2. We can thus summarize as

$$(measured\ by\ simulation) = 2n_k^2 + n_k = \langle a^\dagger a a^\dagger a \rangle \quad (4.100)$$

if the simulation is quantum. Note that the value of these expressions is analytically known.

Now, we can ask what we would obtain from the simulation *including the mapping* if it had already become classical. Therefore, we identify $\langle \alpha^* \alpha \rangle = n_{k,cl}$, assigning a classical occupation number to the mode norm squared. For our example we get instead, from the final line in (4.99),

$$(measured\ by\ simulation) = 2n_{k,cl}^2 - n_{k,cl} \quad (4.101)$$

if the simulation is classical. Note the minus sign subtracting the correction term instead of adding it as for the quantum case.

However, this expression is not analytically known. Only if the simulation has fully thermalized, or if we started with a classical equipartition sampling and considered the classical two-mode squeezed state as in Chapter 2, were we able to predict these numbers with ease. But we start the simulation with the quantum sampling from the Bose-Einstein Wigner function, and are interested in relatively short evolution times without full thermalization. Without having a prediction for *both* the quantum case *and* the nonequilibrium classical ensemble at any time in the simulation we can hardly decide which state the simulation is in as a mere departure from the quantum value then cannot be quantified. We are thus looking for more direct evidence than just a difference in numbers.

Clearly, for small enough $\langle \alpha^* \alpha \rangle$, the squared term in (4.101) can be neglected and the classical result is negative, while it should be positive if the simulation was still quantum according to (4.100). The threshold is $\langle \alpha^* \alpha \rangle \leq 0.5$. This is the same threshold for which a much simpler observable also indicates that the simulation became classical, which is $\langle a^\dagger a \rangle = \langle \alpha^* \alpha \rangle - 0.5$. Indeed, for $\langle \alpha^* \alpha \rangle \leq 0.5$, the TWA-calculated occupation number itself clearly becomes negative and thus shows a transition to the classical regime. This is indeed observed for modes with large enough wave number compared to the temperature.

Extrapolating the discussed example would suggest that unless one looks for low occupation numbers, it may be very difficult to answer the question about the classicality of the simulations by simple means of occupation numbers, quite similar to the experimental situation explained in the first part.

5. Implementation

5.1. Integration of the GPE

5.1.1. Evaluation of the right hand side

With an external potential $\bar{V} = \bar{V}(\bar{x})$, the dimensionless PGPE for the Fourier transformed field $\bar{\psi}_{\bar{k}} = \mathcal{F}[\bar{\psi}(\bar{x})]$ with the projector implemented as a Fourier space cutoff¹ reads

$$i\partial_{\bar{t}}\bar{\psi}_{\bar{k}} = \frac{\bar{k}^2}{2}\bar{\psi}_{\bar{k}} + \mathcal{PF}\left[\left(\bar{V}(\bar{x}) + C_{nl}|\bar{\psi}(\bar{x})|^2\right)\bar{\psi}(\bar{x})\right] \quad (5.1)$$

where $\mathcal{F}$ is the Fourier transform, $\bar{\psi}(\bar{x}) = \mathcal{F}^{-1}[\bar{\psi}_{\bar{k}}]$, and $\mathcal{P}$ is the projection equivalent to setting Fourier modes above a cutoff to zero (c.f. equation (A.6)).

The kinetic term generating a free evolution can be absorbed for each evolution step from $t = t_0$ to $t = t_0 + t_S$ and thus be explicitly solved for by a transformation to an instantaneous rotating frame $\bar{\psi}'_{\bar{k}} \equiv \exp\left(i\bar{k}^2(t - t_0)/2\right)\bar{\psi}_{\bar{k}}$,

$$\partial_{\bar{t}}\bar{\psi}'_{\bar{k}} = \exp\left(i\bar{k}^2(t - t_0)/2\right)\mathcal{PF}\mathcal{G}\left[\exp\left(-i\bar{k}^2(t - t_0)/2\right)\bar{\psi}'_{\bar{k}}\right], \quad (5.2)$$

where $G[\phi_{\bar{k}}] \equiv -i\left(\bar{V}(\bar{x}) + |\bar{\phi}(\bar{x})|^2\right)\bar{\phi}(\bar{x})$. Resolving fast oscillations explicitly is numerically advantageous.

¹Assuming a sufficiently flat potential, low energy modes are slowly varying and have small high-frequency components.

0				
1/2	1/2			
1/2	0	1/2		
1	0	0	1	
	1/6	1/3	1/3	1/6

Table 5.1.: Butcher tableau of RK4

5.1.2. Time Integration

The field is advanced forward in time using the well-known fourth-order Runge-Kutta method “RK4” with Butcher tableau given in Table (5.1). This algorithm has the advantage compared with some other methods (e.g. split step) that it is trivially compatible with the projector. Here the left column represents at which fractions of one basic time step t_S the right hand side is to be evaluated. This involves four substeps for this particular algorithm. The lower row specifies how these four evaluations are to be linearly combined to obtain the final answer which is to be added to the field to evolve it from t to $t + t_S$. The right hand side of a differential equation depends on the field itself, and in general linear combinations of the previous substep results are used to predict a corrected field as the input for the current substep. The coefficients of this combination are given for each step by the rows of the main body of the table.

When applied to the equation (5.2), we find the following algorithm, with $\psi'_0 = \bar{\psi}'_{\bar{k}}(t = t_0) = \bar{\psi}_{\bar{k}}(t_0)$ (since the frame was assumed to be locally rotating starting at t_0):

$$\Delta_1 = \mathcal{PFG} [\psi'_0] \quad (5.3)$$

$$\Delta_2 = \exp \left(i\bar{k}^2 t_S / 4 \right) \mathcal{PFG} \left[\exp \left(-i\bar{k}^2 t_S / 4 \right) (\psi'_0 + t_S \Delta_1 / 2) \right] \quad (5.4)$$

$$\Delta_3 = \exp \left(i\bar{k}^2 t_S / 4 \right) \mathcal{PFG} \left[\exp \left(-i\bar{k}^2 t_S / 4 \right) (\psi'_0 + t_S \Delta_2 / 2) \right] \quad (5.5)$$

$$\Delta_4 = \exp \left(i\bar{k}^2 t_S / 2 \right) \mathcal{PFG} \left[\exp \left(-i\bar{k}^2 t_S / 2 \right) (\psi'_0 + t_S \Delta_3) \right] \quad (5.6)$$

$$\bar{\psi}_{\bar{k}}(t = t_0 + t_S) = \exp \left(-i\bar{k}^2 t_S / 2 \right) (\psi'_0 + (\Delta_1/6 + \Delta_2/3 + \Delta_3/3 + \Delta_4/6)t_S) \quad (5.7)$$

In the final step it is necessary to rotate back such that the algorithm may be repeated for the subsequent time step $t + t_S \rightarrow t + 2t_S$ with $\psi'_0 = \bar{\psi}_{\bar{k}}(t = t_0 + t_S)$ as the input field.

The algorithm can be rewritten in an optimized way by shifting to another rotated frame. When we redefine the previously used symbols Δ_n and ψ' such that we may replace $\psi'_0 \rightarrow \exp \left(i\bar{k}^2 t_S / 4 \right) \psi'_0$ (implying that the new $\psi'_0 \equiv \exp \left(-i\bar{k}^2 t_S / 4 \right) \bar{\psi}_{\bar{k}}(t_0)$!), $\Delta_1 \rightarrow \exp \left(i\bar{k}^2 t_S / 4 \right) \Delta_1$, $\Delta_2 \rightarrow \exp \left(i\bar{k}^2 t_S / 4 \right) \Delta_2$, $\Delta_3 \rightarrow \exp \left(i\bar{k}^2 t_S / 4 \right) \Delta_3$, $\Delta_4 \rightarrow \exp \left(-i\bar{k}^2 t_S / 2 \right) \Delta_4$, we get

$$\Delta_1 = \exp \left(-i\bar{k}^2 t_S / 4 \right) \mathcal{PFG} [\psi_0] \quad (5.8)$$

$$\Delta_2 = \mathcal{PFG} [\psi'_0 + t_S \Delta_1 / 2] \quad (5.9)$$

$$\Delta_3 = \mathcal{PFG} [\psi'_0 + t_S \Delta_2 / 2] \quad (5.10)$$

$$\Delta_4 = \mathcal{PFG} \left[\exp \left(-i\bar{k}^2 t_S / 4 \right) (\psi'_0 + t_S \Delta_3) \right] \quad (5.11)$$

$$\bar{\psi}_{\bar{k}}(t = t_0 + t_S) = \exp \left(-i\bar{k}^2 t_S / 4 \right) \{ \psi'_0 + (\Delta_1/6 + \Delta_2/3 + \Delta_3/3)t_S \} + \Delta_4/6 t_S. \quad (5.12)$$

Here, in the first equation we made use of $\psi'_0 = \psi_0$ before changing the definition of ψ'_0 , that is, Δ_1 is computed starting from the unprimed output field from the last timestep. This reduces the amount of 7 multiplications with the various free evolution phase factors to only 4 multiplications all with the same factor $\exp \left(-i\bar{k}^2 t_S / 4 \right)$ (including the one to obtain ψ'_0), giving performance as well as memory access advantages.

5.2. The BECS Software

BECS is a software package written in C (core), Python (task scheduler) and Matlab (data analysis and visualization), that can simulate a homogeneous BEC with variable interaction strength in two and three dimensions using PGPE and TWA methods.

It is based on Matlab code written by Piyush Jain and Silke Weinfurtner for two dimensions and uses the same core algorithms. However, it was optimized for maximal performance and ease of use, and contains several extensions.

The core algorithm has been rearranged, and great care has been taken with memory use and memory alignment of the simulated fields and auxiliary variables. No unnecessary calculations are performed in view of the projector.

As a consequence, single trajectories run slightly faster compared with Matlab's matrix computations on a standard machine of 2015. The main speed-up is achieved when multiple trajectories run in parallel. Since the new programme is so small and strictly uses only one core, 16 trajectories run 16 times as fast as a single trajectory on a 16 core server. With Matlab, the server would have been saturated once a few copies of the software run at the same time. This means that BECS runs about 10 times faster in practice than the old Matlab code.

BECS has also been ported to CUDA C to execute its core on Nvidia graphics cards. The author has not seen this improving the performance on his laptop, but on future workstations with special computing graphic accelerators this could provide useful for speeding up single trajectories.

Furthermore, the data analysis section has been totally rewritten. The stochastic average to determine correlators is done by another, fast, C tool and the results are saved in binary to be quickly imported into Matlab. This makes the analysis and data visualization code run without notable delay for many reasonable data set sizes. As a consequence, instead of having to wait minutes for a few noisy data points, we can now view smooth trajectories immediately. In addition, the tool can average over arbitrarily large datasets saved on the

hard disk without needing the corresponding amount of RAM at the same time. Some datasets in this thesis are larger than 100GB, so this is a crucial improvement. Finally, the observables from Section 4.2.3 have been implemented.

For instructions how to install and use BECS refer to Appendix B

5.3. Simple Test Cases

5.3.1. Convergence

Using a fourth order Runge-Kutta algorithm for integrating in time, we expect that the error roughly scales with the step size t_S^5 . To check this, we investigate the extent of numerical particle number (norm) conservation for relatively short single trajectory runs as a function of t_S . In theory, norm conservation strictly follows from the form of the GPE just like for the Schrödinger equation. We leave the interaction strength constant in time, and choose the experimentally typical total atom number $N_0 = 1 \times 10^7$. The initial state is thermal with $T = 2C_{nl}$ (see Chapter (A.1)). There is no random noise for the PGPE simulations, but the quasiparticle modes are occupied deterministically with the equipartition distribution $n_k = T/\omega_k$.

Cases of different grid sizes and grid dimensions are investigated for three different values of the nonlinearity scale C_{nl} of 10000 to 30000, which are for these test cases all relatively high such that interesting effects beyond Bogoliubov theory can appear for sufficiently long times, but not for shorter times.

In all test cases we find that after an initial, typically very short period of time, the norm changes linearly in time, and we can directly assign a norm error rate r , which is the particle number change per unit time relative to the total particle number.

These rates r are shown in table 5.2 for all three values of C_{nl} for the case of a 128^2 grid. Time steps so large that the simulation does not make sense have not been included. The number of time steps calculated is varied from case to case to ensure a total simulation time long enough for accurately assigning the error rate r .

Table 5.2.: Relative norm error rates

$10^6 \times t_S$	$C_{nl} = 1 \times 10^4$	$C_{nl} = 2 \times 10^4$	$C_{nl} = 3 \times 10^4$
0.5	0.0021	0.13	1.5
1	0.066	4.2	48
2	2.1	133	1.5×10^3
4	66	4.0×10^3	4.1×10^4
8	2.0×10^3	9.7×10^4	-
16	4.86×10^4	-	-

The rates for these and other test cases are plotted double-logarithmically as a function of time step size in figure (5.1), and linear fits have been obtained for each case. We find the linear fits to have slope 4.8 to 4.9. This establishes that the fourth order algorithm is implemented correctly.

Simulations on a 3D grid with size 32^3 have also been carried out, but they lie exactly on those of the 128^2 grid in 2D for all three values of C_{nl} . It is noted that the mode numbers in the projected region are similar but not the same in these cases (they are 2109 in 32^3 and 3209 in 128^2). The number of modes in a bounding box of the projected region, which is 16^3 in 3D and 64^2 in 2D, is 4096 in both cases, however, which may be the reason for this equivalence.

Despite the cases shown in figure (5.1), simulations were also run at a lower temperature of $T = C_{nl}$. For the 128^2 cases for all values of C_{nl} we find again that this does not affect the results. For the other grids, a lower temperature helps norm conservation and shifts the linear graphs to the right (not shown).

5.3.2. Thermalization

As noted in passing in Section 4.2.4, each individual TWA trajectory is equivalent to a PGPE run (with some initial noise). In the long time limit, the occupation numbers will thus approach the classical equipartition distribution for the quasiparticles in the quadratic theory

instead of the Bose-Einstein distribution in the sense of a microcanonical time-ensemble average. Averaging over the TWA ensemble consisting of different draws from the Wigner function and different energies is expected to give the same results in the same way that the canonical ensemble will give the same results as the microcanonical ensemble. The different energies are negligible and the initial set-up for the different trajectories are like starting at random positions in phase space of the same microcanonical situation. If this initial set-up is not the equilibrium state, we are interested in following the time evolution of observables. It is then good to have an ensemble average given by averaging over many trajectories at a given time instead of having to do a time average, which washes out the average behaviour of observables in time. It is much easier to see if the system has thermalized with this approach than when following a single trajectory which will show chaotic behavior even in equilibrium.

2D

For $C_{nl} = 30000$ we have started with a Gaussian thermal state and evolved until $\bar{t} = 1$, which is 625000 time steps to keep the error in norm conservation extremely low. The initial state is not exactly the thermal state for the quantum system with a square root of the depletion of roughly 6%. This observable is also useful to estimate how much a simulation has thermalized. We see in Fig. 5.2 that actually thermalization does not seem complete, as the depletion still seems to show a falling trend. Note that since this is a microcanonical simulation it will never be stationary even in equilibrium.

Interestingly, for the highly occupied low momentum modes in the top of Fig. 5.3 the state does not behave totally Gaussian. The departure from Bogoliubov theory is already obvious for these modes. However, as the simulation thermalizes and the mode occupation drops, the non-Gaussianity also decreases.

Despite not having reached equilibrium yet, equipartition can be seen to be satisfied for the ultraviolet modes in Fig. 5.4. In the infrared the modes are still occupied too much despite a correction with the modified dispersion relation beyond Bogoliubov measured as described in Section 4.2.3.

Note that the value for C_{nl} chosen here is higher than what we discovered to be experimentally feasible in two dimensions in Section A.2.2, and yet thermalization takes a long time.

It is curious that in the end of the simulation time when thermalization may be just reached, the non-Gaussianity just about vanishes. A priori, Gaussianity is not expected in the thermal state for high depletion. If we can say that for this amount of depletion we do expect an almost Gaussian thermal state, the initial non-Gaussianity might indicate that unbalanced scattering is happening which leads to a redistribution of mode occupation.

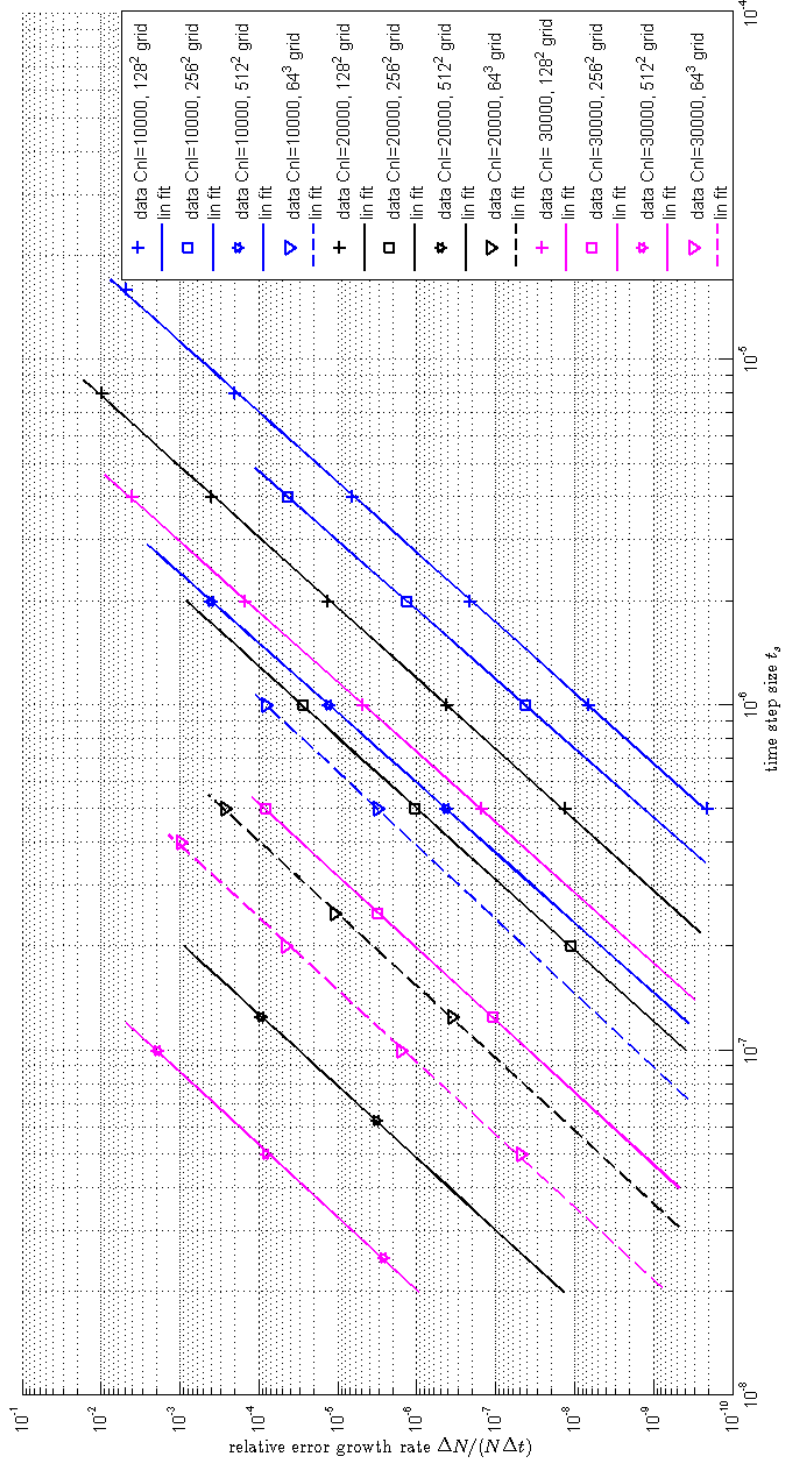


Figure 5.1.: Double logarithmic plot of the particle number error rate in free evolution as a function of step size for the indicated test cases. The straight lines are linear fits through the data.

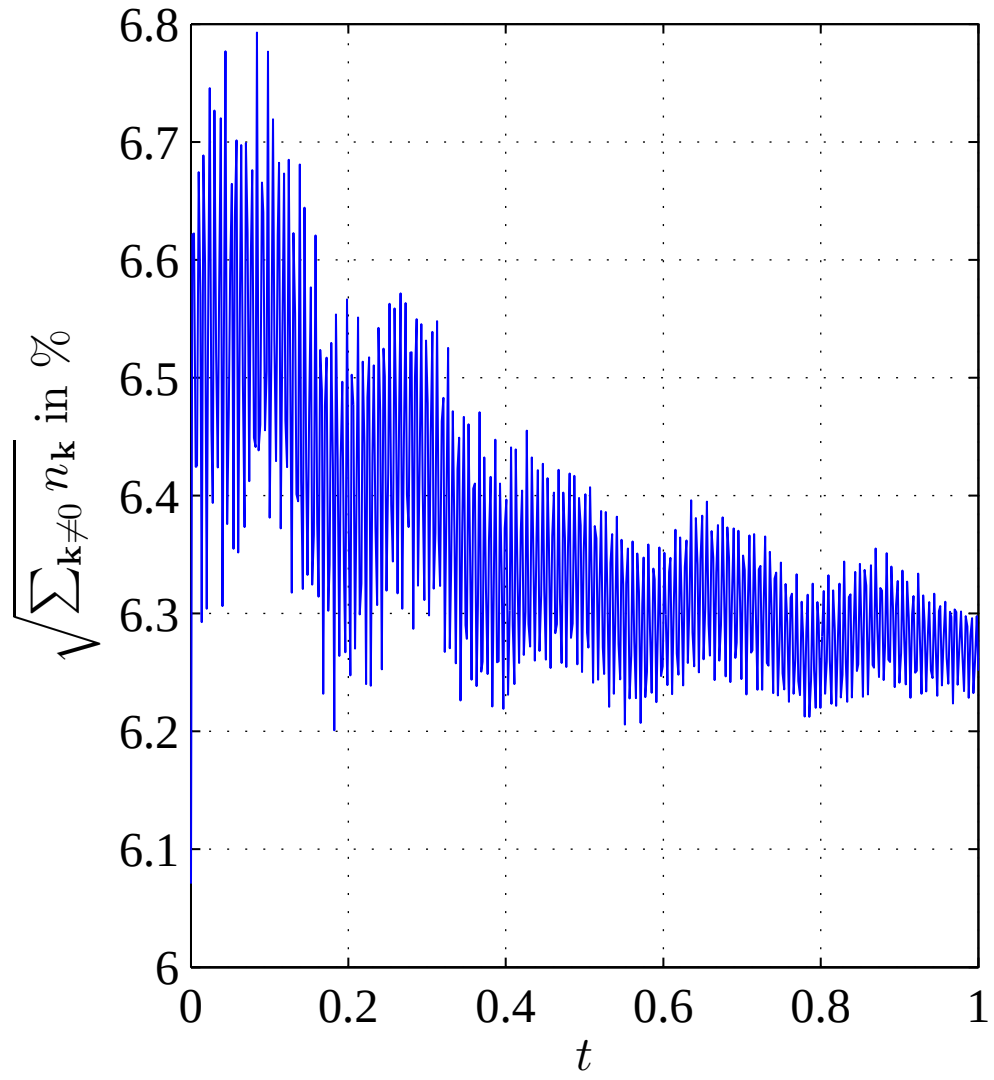


Figure 5.2.: Evolution of the square root of the depletion.

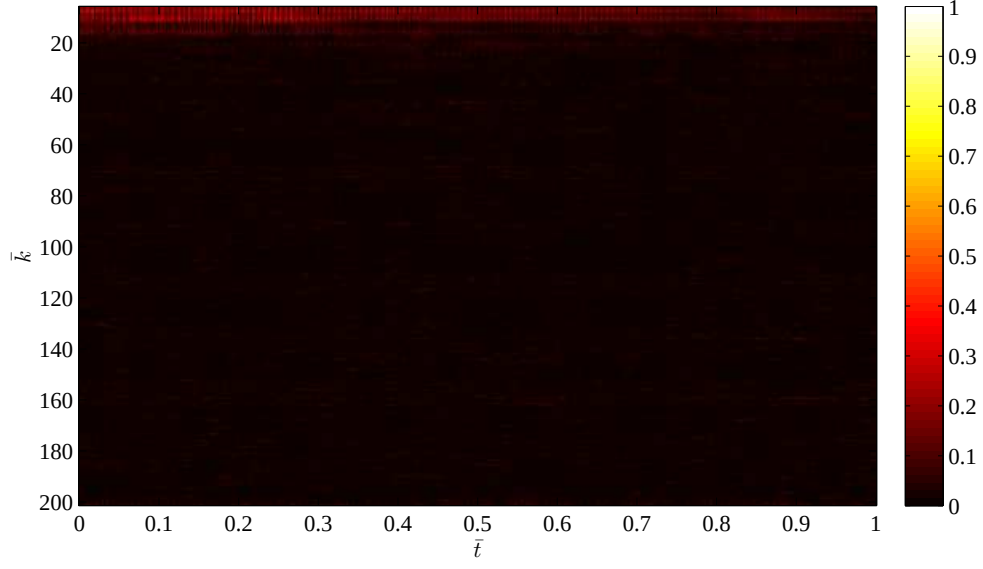


Figure 5.3.: Nongaussianity in the lowest modes.

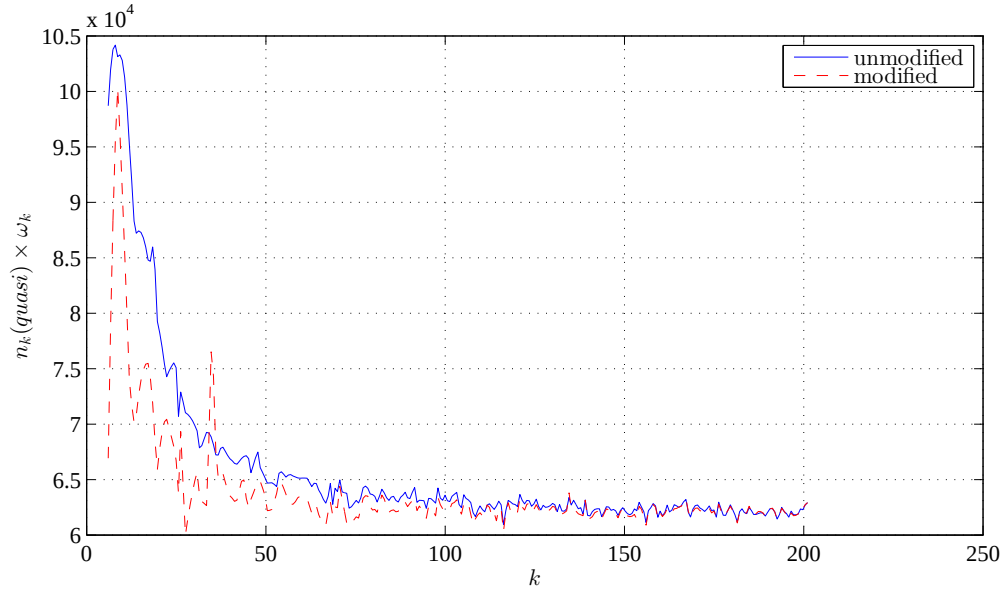


Figure 5.4.: With the modified dispersion relation, the result is slightly closer to equipartition.

6. Results

6.1. Parametric Resonance

We run a $N = 64^3$ cubic grid simulation with $C_{nl}(t = 0) = 10000$ until $\bar{t} = 0.08$ with a time step of $t_S = 1e^{-6}$, sufficient as seen in chart (5.1). There are 40 periods of a square wave oscillation of the interaction strength by 20% implying 80 total jumps of C_{nl} to 12000 and back. The period is calculated such that a set of grid modes with $\bar{k} = 10\pi$ are hit exactly with the resonance according to formula (1.44). This gives a total time of the square wave modulation of 0.0396, i.e. slightly less than half the total simulation time. The modulation is started in the beginning. We expect the growth of resonance peaks in the first half of the simulation.

We present some observables for 48 averaged trajectories. For the occupation number, we compare to the exact theoretical prediction. Agreement is exceptionally good initially as seen in Fig. 6.1 which shows the occupation number of the real particles' first resonance mode. After about half the time the modulation stops. Decay channels become visible in the simulation (Fig. 6.2), which are absent in the quadratic Bogoliubov theory-based calculation (Fig. 6.3) and should not be confused with the direct excitation of the harmonics, which *are* covered by Bogoliubov theory. Note that the excitation of harmonics is more an artefact of the parametric excitation type than of using a square signal, as even with a sinusoidal modulation these peaks are expected.

The peaks are also slightly shifted to lower values of k . This could simply be a discretization artifact on the grid. However, there are other grid nodes at higher k which match the resonance condition better. This shift has been corrected for in Fig. 6.1.

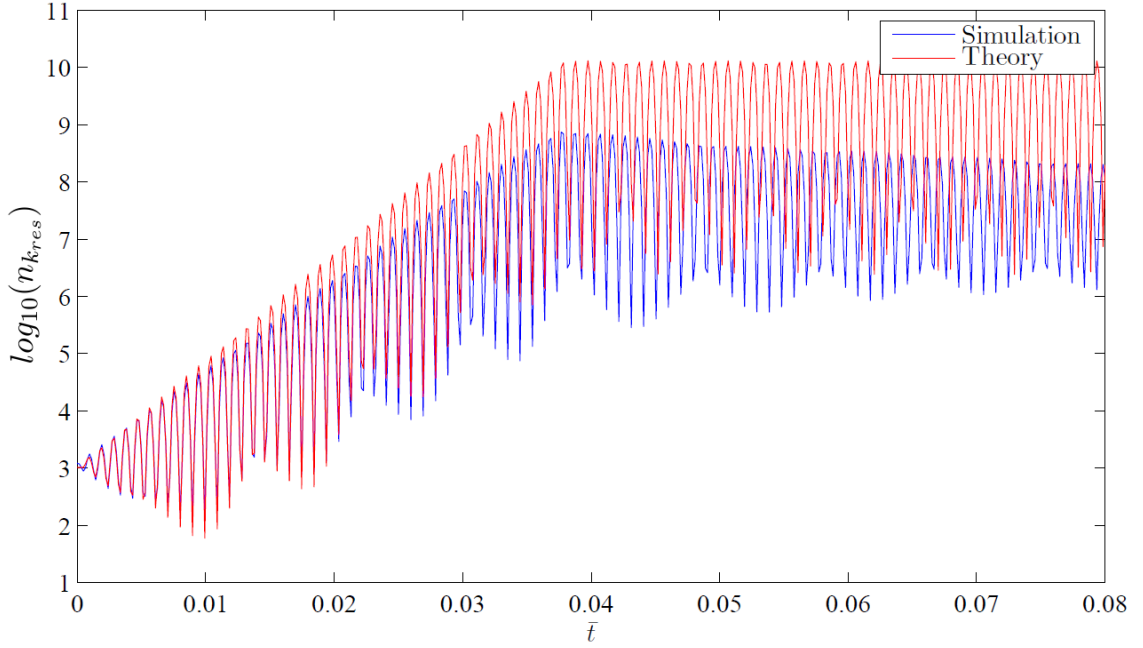


Figure 6.1.: Formation of the main resonance peak for parametric driving. The occupation number of the real particles is plotted in logarithmic scale for simulation and theory. Agreement is excellent for the first six oscillations of the mode. The simulation includes decay effects, which reduce the growth rate early on.

Next, we have a look at the TMV as predicted by the simulation in Fig. 6.4. Sub-Poissonian statistics occur at both peaks after sufficient driving, but disappear soon after when the peaks get large enough to begin scattering into other modes.

The result is compatible to the theoretically equivalent CSI violation shown in Fig. 6.5: blue sub-Poissonian regions correspond to black CSI-violating regions. However, when compared with the full Gaussian entanglement criterion from the covariance matrix in Fig. 6.6, it is seen that mode entanglement is in this set-up with scattering contributing to the physics not perfectly determined by TMV and CSI, as now the entangled regions are significantly smaller.

Finally, we check if we can fully trust the last criterion by checking Gaussianity of the state in Fig. 6.7. Interestingly, there are strong departures from Gaussianity for modes with scattering. Thus, the entanglement as shown in Fig. 6.6 may not be sufficient. However,

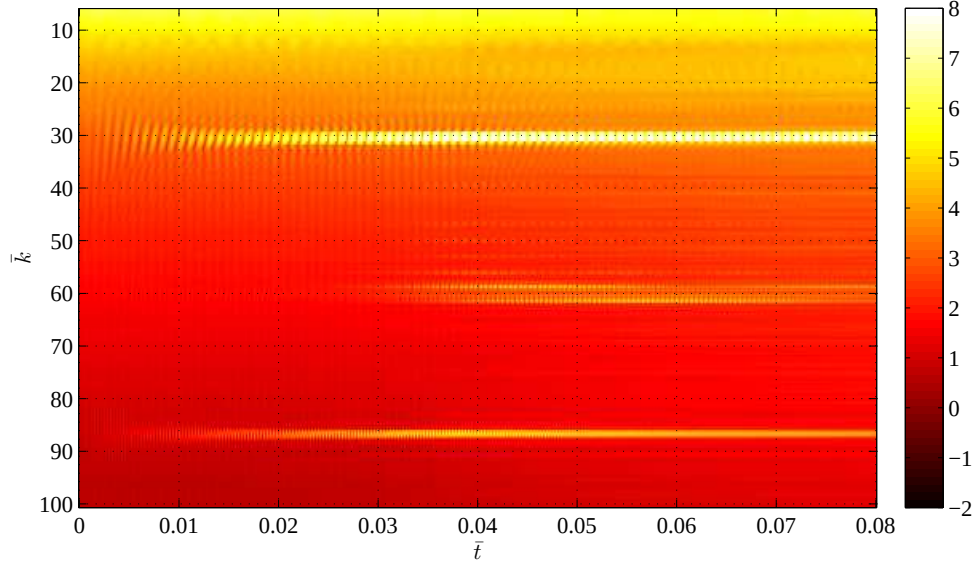


Figure 6.2.: Result from simulation for $\log_{10} n_k$ for the same parametric setup as before.

One can see decay channels that excite further modes absent in the analytical calculation, where phonon interactions are neglected.

there is no reason to believe that the CSI and TMV are better criteria in the non-Gaussian case even though the “entangled” regions are appearing bigger.

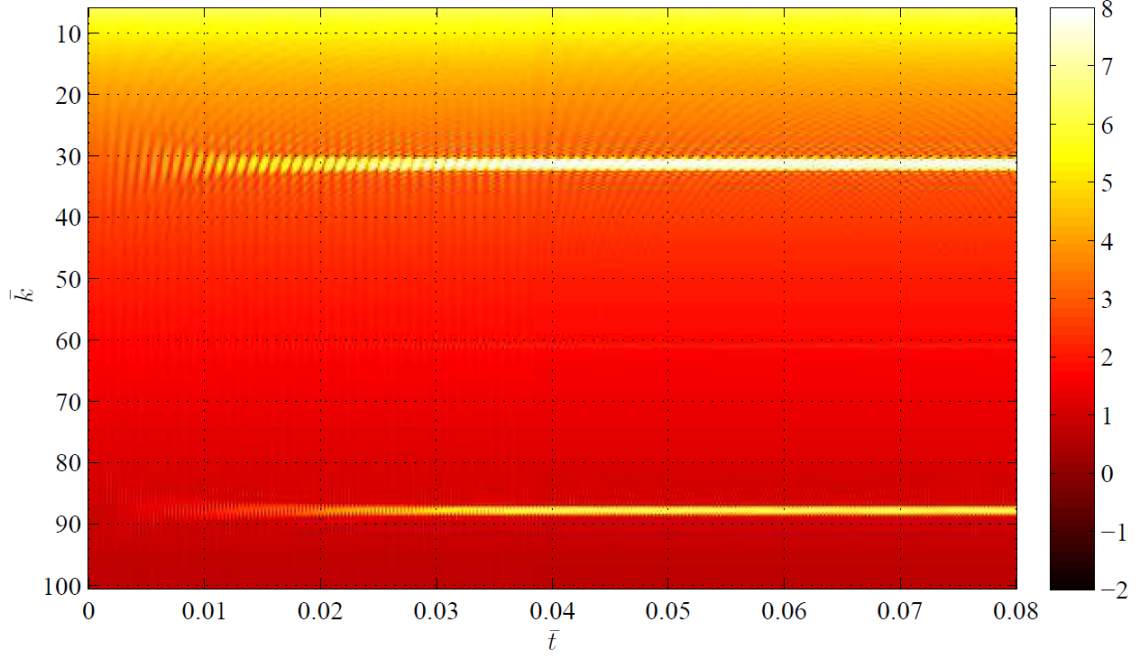


Figure 6.3.: Analytical prediction for $\log_{10} n_k$ showing the parametric excitation of first and third harmonic by a square wave driving.

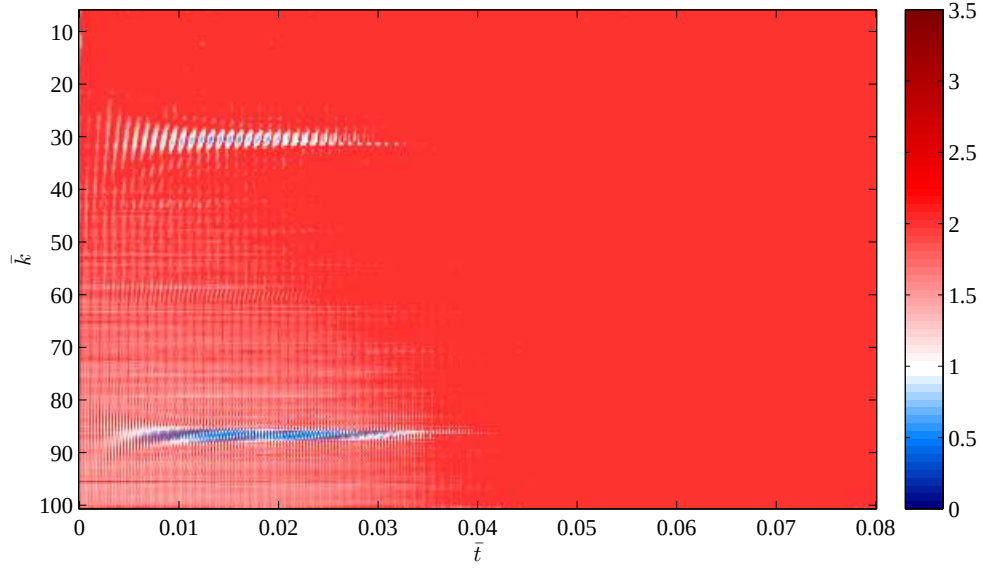


Figure 6.4.: TMV for parametrically excitations as measured by the simulation.

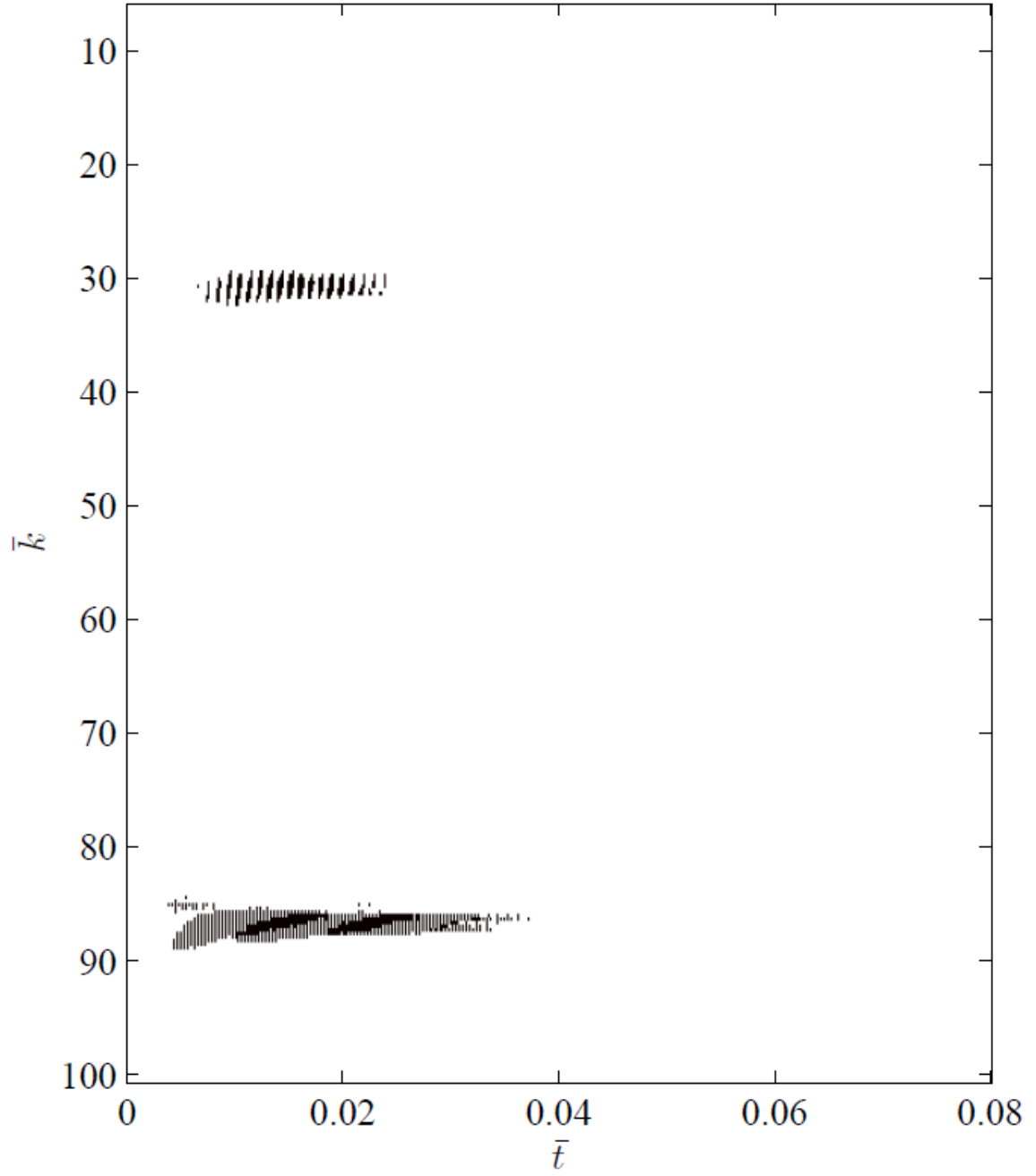


Figure 6.5.: The CSI violation (black) appearing in the first and third harmonic is comparable to the TMV criterion.

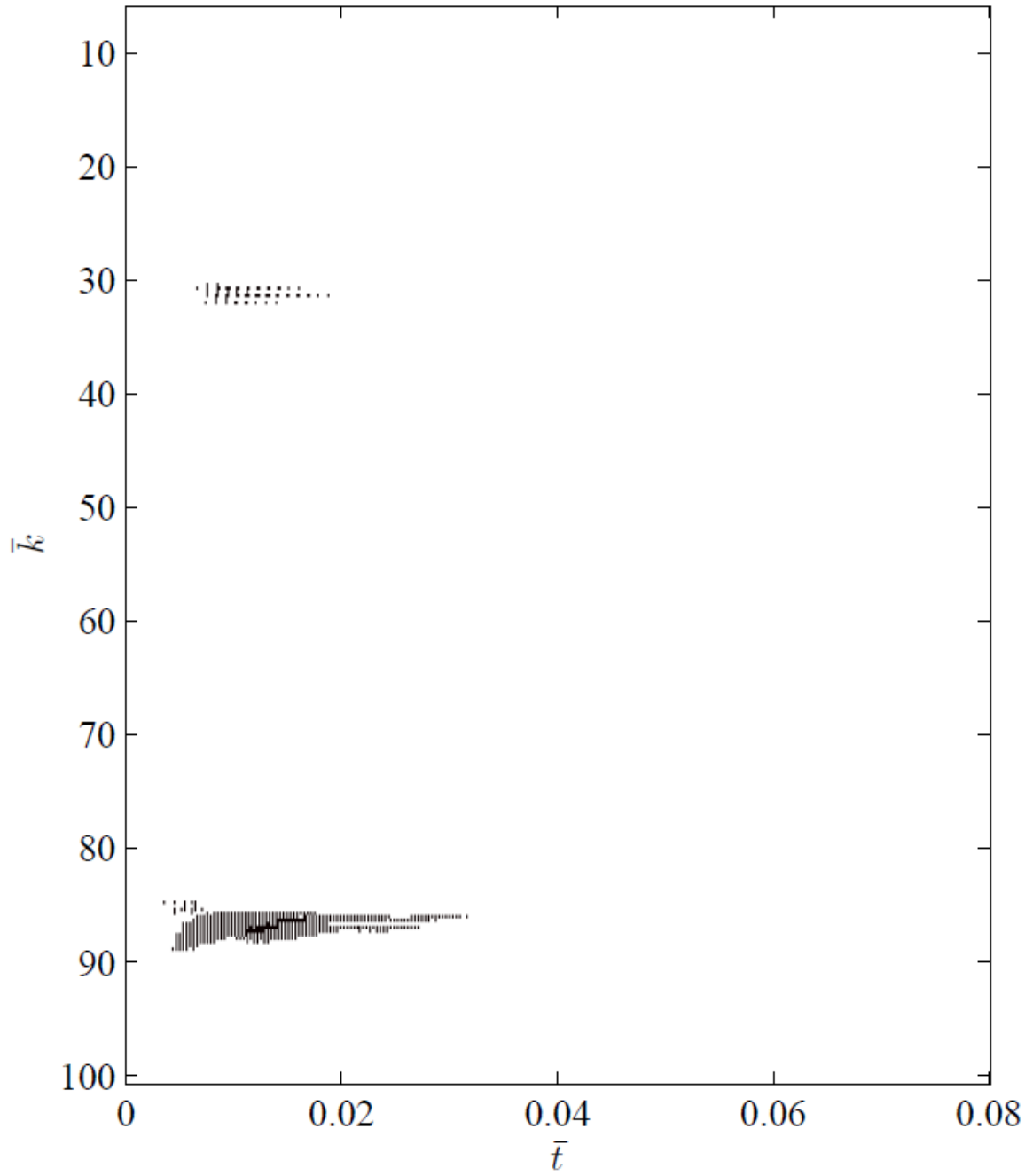


Figure 6.6.: In the $k - t$ plane, regions of nonseparability (black) appear as a subset of the CSI violation in the simulation due to effects beyond Bogoliubov theory.

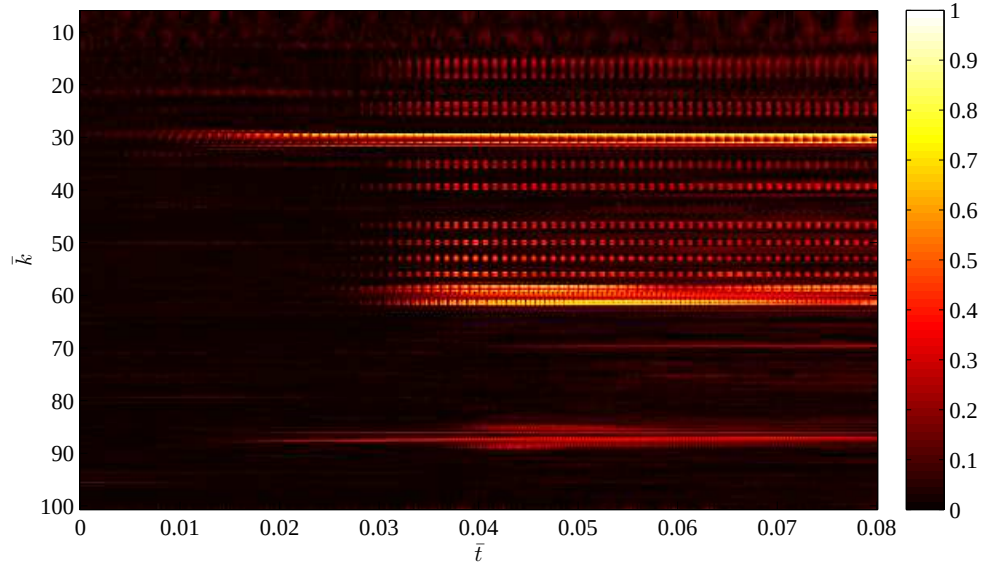


Figure 6.7.: Test of mode-specific Gaussianity of the state for the parametrically excited condensate as simulated by TWA. The closer the value is to zero, the closer the state is to be Gaussian w.r.t. the mode.

7. Conclusions of Part III

We have in this part of the thesis introduced the reader to the theory of TWA simulations and its practical implementation with focus on the evaluation of nonclassicality criteria. The implementation of TWA developed by the author was tested for the parametric resonance studied in this thesis since we can compare to exact analytical results in this nontrivial setting. Excellent agreement was achieved on time scales where phonon-phonon interactions are not relevant.

The distinction of quantum and classical simulations is seen to be even more difficult than for the theoretical considerations in the first part. First, the difficulties uncovered there for the definition of a strong nonclassicality criterion for experiments directly apply to the simulations as well. Classical simulations correspond to the classical reference introduced above and can also violate intensity CSI and show sub-Poissonian statistics. Furthermore, for the TWA simulations the quantum aspects of the numerical results consist out of two parts, one simply due to operator ordering corrections and one due to sampling statistics. We have attempted to develop an operational distinction with the goal to test the time-scale of the validity of TWA but more work is necessary to understand this better.

There are further directions that can be explored with the simulations. One such topic is the influence of dimensionality. We have carried out 2D simulations on grids of size 256^2 . The results are very similar to those in 3D. A difference is that damping effects are weakened. Another interesting topic is that of vortex formation. By plotting the phase of the real-space condensate we have observed the formation of vortices binding to vortex pairs for initial states of high depletion in few low momentum modes (corresponding to the collision of multiple condensates).

Starting with a thermal state, it seems from our investigations impossible to create vortices from parametric resonance, unless perhaps when the driving is so strong as to completely destroy the condensate, which leads to a chaotic behavior of the phase.

From the theoretical side there is also opportunity for further work to a) understand the derivation of TWA from the path integral in a completely rigorous way including the prefactor of the operator expectation values by taking the continuum limit after the Wigner-Weyl transforms, b) to investigate rigorously what the conditions are that the semi-classical approximation, which generalizes the GP equations by introducing a coupled second field, reduce to the purely classical GPE evolution, and c) to investigate possible generalizations of the TWA method to this complete set of equations.

A. Units and Parameters

A.1. Dimensionless Rescaling

Since $\hbar$ has units of energy $\times$ time or momentum $\times$ length, $\hbar^2/m$ has units of energy $\times$ length-squared. Thus, given any length scale r_0 , we can associate to it an energy $E_0 = \hbar^2/(mr_0^2)$ and a time $T_0 = \hbar/E_0$.

Factoring out E_0 from any kinetic energy term $\hbar^2 k^2/2m$ leaves $\bar{k}^2/2$ with dimensionless $\bar{k} = kr_0$. In this chapter, the bar will indicate that a quantity is dimensionless.

For theoretical studies of BECs, and in particular systems of infinite size, the length scale r_0 may be chosen to be the healing length $\xi = \hbar/\sqrt{Umn}$ (our definition is larger by a factor of $\sqrt{2}$ than a more common definition for the gas in the box, and we have used the condensate number density n instead of the total number density n_0). With this choice, the energy scale is set by the interactions, $E_0 = Un$, and the dispersion relation (1.5) reads $\bar{e}_k = e_k E_0^{-1} = \sqrt{\bar{k}^2/2 \times (\bar{k}^2/2 + 2)}$. Thus, modes with $\bar{k} = 2$ are situated at the crossover between phononic and free particle regime, since both terms under the square root have the same value. Note that this is not exactly equal to the mode corresponding to the healing length, which is $\bar{k} = 2\pi$.¹ Since the dimensionless version of ω_k is $\bar{\omega}_k = \bar{e}_k$, the speed of sound in $\bar{\omega}_k^2 = \bar{c}^2 \bar{k}^2 + \mathcal{O}(\bar{k}^4)$ is $\bar{c} = \sqrt{2}/2$ for these units. Due to removing the inherent interaction energy scale by this particular choice of units it is possible to interpret one plot of results as being valid for all interaction strengths. The actual inverse length of, say, a

¹For this to be true, one would have to define the healing length $\xi' = \pi\xi$ being even larger by a further factor of π regardless of the units used (with $r_0 = \hbar/\sqrt{Umn}$ unchanged, the transition would still occur at $\bar{k} = 2$, which corresponds to a wave vector of $k = 2/r_0 = 2\pi/\xi'$ indeed).

Table A.1.: Conversion of unit systems used in this thesis

	thesis units $r_0 = \xi$	simulation units $r_0 = L$
energy	E	$C_{nl}E$
wave vector	$\bar{k}$	$\bar{k}\sqrt{C_{nl}}$
phononic regime	$\bar{k} < 2$	$\bar{k} < 2\sqrt{C_{nl}}$
time	$\bar{t}$	$\bar{t}/C_{nl}$

particular momentum mode, then depends on the unspecified interaction energy through the healing length ξ . We use these units in all theoretical plots in this thesis.

On the other hand, for experiments and simulations the system size is also convenient as a scale to which other quantities can be related, $r_0 = L$. Then, a mode with $\bar{k} = 2\pi$ corresponds to the de Broglie wavelength of $\lambda = 2\pi/k = L$. This means that in a box of length L , the dimensionless wave vector $\bar{k}$ has the interpretation of a mode number (times 2π) in a Fourier series expansion.

With the latter choice of $E_0 = \hbar^2/(mL^2)$, we define the dimensionless ratio

$$C_{nl} := \frac{Un}{E_0} \frac{N_0}{N}, \quad (\text{A.1})$$

where N_0 is the fixed total atom number of the system and the subscript nl stands for *nonlinear* for reasons that will become clear shortly. Since $n = N/V$ (as occurring in the dispersion relation) is referring to the density of the condensate part only, C_{nl} is independent of the depletion. The dispersion relation then reads $\bar{e}_k = \sqrt{\bar{k}^2/2 \times (\bar{k}^2/2 + C_{nl} N/N_0)}$.

However, since we focus on the Bogoliubov regime, we are ignoring the next-order N/N_0 correction and N may as well refer to the total atom number.

By definition, C_{nl} is the factor transforming between the two energy scales of the two unit systems that have been introduced, and conversions of modes and times follow as summarized in table (A.1).

Note here that even if the system is contained in a planar shape and effectively two-dimensional, scattering is assumed to take place in three dimensions. The quantity $n = N/V$

may be always understood as the 3D density (in a trapped inhomogeneous system, locally $n(x) = \delta N / \delta V$).

With $U = 4\pi\hbar^2 a / m$ expressed in terms of the scattering length, we have $C_{nl} = 4\pi a N_0 L^2 / V$. For 3D and 2D this comes out to be, respectively,

$$C_{nl} = 4\pi N_0 a / L \quad \text{in 3D} \quad (\text{A.2})$$

$$C_{nl} = 4\pi N_0 a / L_z \quad \text{in 2D}, \quad (\text{A.3})$$

where in 2D we have assumed a box shape of $L \times L \times L_z$.

In the GPE there is a nonlinearity term $U|\psi|^2\psi$, and $U|\psi|^2$ must have units of energy. Dividing this by E_0 gives with the definition of C_{nl} in (A.1) the nonlinearity term $C_{nl}|\psi|^2\psi/V/N_0$. Note that ψ itself has units of $V^{-1/2} \equiv L^{-d/2}$. We then introduce a dimensionless, normalized field as a function of the dimensionless coordinates by absorbing the V/N_0 factor in $|\psi|^2$ (any arbitrary factor that just remains in the linear ψ is irrelevant and can be divided out of the equation)

$$\bar{\psi}(\bar{x}) := \psi(\bar{x}L)L^{3/2}N_0^{-1/2} \quad \text{in 3D}, \quad (\text{A.4})$$

$$\bar{\psi}(\bar{x}) := \psi(\bar{x}L)(L^2L_z)^{1/2}N_0^{-1/2} \quad \text{in 2D}. \quad (\text{A.5})$$

With this definition, the interaction term in the GPE becomes simply $C_{nl}|\bar{\psi}|^2\bar{\psi}$, and the normalization is $\int |\bar{\psi}(\bar{x})|^2 d^3\bar{x} = \int |\psi(x)|^2 d^3x / N_0 = 1$.

Explicitly, the dimensionless PGPE then reads

$$i\partial_t \bar{\psi} = \frac{\nabla^2}{2} \bar{\psi} + \mathcal{P} \left[\left(\bar{V}(\bar{x}) + C_{nl}|\bar{\psi}(\bar{x})|^2 \right) \bar{\psi}(\bar{x}) \right], \quad (\text{A.6})$$

with the projector $\mathcal{P}$ introduced in Section 4.1 and explained in Subsection 5.1.1.

For a discrete representation of $\bar{\psi}$ in a 3D box with grid size $\mathcal{N}$ in each Cartesian direction, the volume element is simply $d^3\bar{x} = \mathcal{N}^{-3}$. In 2D, one side of the box corresponding to L_z is represented by a single layer, and the volume element is $d^2\bar{x} = \mathcal{N}^{-2}$. In both cases, the integrals reduce to averaging sums over the grid.

For 2D, we have effectively assumed that the field is constant in z -direction. A more careful treatment assumes a harmonic oscillator ground-state like Gaussian profile in z -direction with

z -dependent width to be determined by minimizing the usual semiclassical action [Salasnich et al., 2002]. In the 2D regime

$$\mu, k_B T \ll \hbar \omega_z \quad (\text{A.7})$$

with a harmonic trapping frequency of ω_z in z -direction, this yields an effective description by a 2D GPE with an interaction term with interaction strength $U_{2D} = 2\sqrt{2\pi}\hbar^2/ma/L_z$. In this case, $L_z^2 := \hbar/m\omega_z$ is understood precisely as the length giving the spread of the wave function of the harmonic potential ground state. Note that with $n_{2D} := N/L^2$, this amounts to a replacement of $Un \rightarrow U_{2D}n_{2D} = Un/\sqrt{2\pi}$. In dimensionless units, the result of the careful treatment is thus a simple numerical correction factor of the result (A.5) above,

$$C_{nl} \equiv \frac{n_{2D}U_{2D}}{E_0} = 2\sqrt{2\pi}N_0\frac{a}{L_z} \approx 5N_0\frac{a}{L_z} \quad \text{in 2D.} \quad (\text{A.8})$$

Importantly and unlike in 3D, with the scattering length a and atom number N_0 fixed, C_{nl} is actually controlled by the transverse trapping frequency, $C_{nl} \propto \sqrt{\omega_z}$ (as is U_{2D}). The first 2D-condition in (A.7), which is approximately (using $\mu \approx U_{2D}n_{2D} = C_{nl}E_0$)

$$C_{nl} \ll E_0^{-1}\hbar^2/mL_z^2 = \left(\frac{L}{L_z}\right)^2 = \frac{\omega_z}{\omega_{xy}}, \quad (\text{A.9})$$

appears to set an upper bound on C_{nl} (and for fixed C_{nl} , it seems to set an upper bound on the thickness L_z). However, it would be wrong to assume that a simulation with higher C_{nl} than another can still be interpreted as valid and simply corresponding to the same gas in a more flat-shaped trap because of the dependence of C_{nl} itself on the thickness. Taking into account expression (A.8) to replace the thickness in terms of C_{nl} , we have

$$\frac{C_{nl}}{N_0^2} \frac{L^2}{a^2} \gg 8\pi \approx 25 \quad (\text{A.10})$$

putting a *lower* bound on C_{nl} when instead of the trap frequency ratio the scattering length a and particle number are taken as fixed. On the other hand, we can get an upper bound on the thickness, if C_{nl} is instead replaced in favor of L_z , as

$$L_z \ll \frac{L^2}{5N_0a}. \quad (\text{A.11})$$

This is a physical condition that could have been directly derived from (A.7) without introducing C_{nl} , and does not make a connection to the simulation parameters. Importantly,

for a given scattering length this shows that for an increase in particle number the transverse thickness has to decrease to stay in the 2D quasicondensate regime, which increases the 3D density dramatically.

A.2. Parameters and Experimentally Feasibility

A.2.1. 3D Simulations

Picking rubidium-87 with a scattering length of $5.2nm$ ($\approx 100a_0$) and $m = 87u$, and assuming a condensate size of $100\mu m$, we get $E_0 = 7.6 \times 10^{-34}J$ and, according to equation (A.2) and further assuming an atom number of $N_0 = 10^7$,

$$C_{nl} = 6500$$

$$\hbar/E_0 = 14s.$$

A higher C_{nl} at fixed atom number can be reached by considering a smaller (and thus denser) system, or, if the system permits, by increasing the interaction strength at a Feshbach resonance. Thus, simulations with the parameters of $C_{nl} = 10000$ and $N_0 = 10^7$ correspond to realistic systems in 3D.

A.2.2. 2D Simulations

A realistic atom number for systems confined to two dimensions is expected to be smaller than the 3D number. We may assume $N_0 = 10^5$ atoms. Then, the thickness is bounded by (A.11) and for the given scattering length of Rubidium-87 for $L = 100\mu m$ we obtain $L_z = \alpha 4\mu m$ with $0 < \alpha \ll 1$, which is already a very flat condensate with $\omega_z/\omega_{xy} \gg 625$. While it appears from (A.9) that $C_{nl} = 625$ (or lower) would then be sufficient, its value is in this setting already fixed from (A.8) to be $625/\alpha$, which is indeed still satisfying (A.9) as it is much smaller than $625/\alpha^2$ of course precisely since $\alpha \ll 1$ is ensuring a full implementation of the 2D condition already. Similarly, condition (A.10) is satisfied since the left hand side is $25/\alpha$.

A particle number larger than $N_0 = 10^5$ would for rubidium-87 demand an unrealistically flat shape and a high 3D density, which would cause a too large 3-body loss rate. On the other hand, in the TWA approach, a lower particle number increases the Wigner noise amplitude with respect to the condensate population. To avoid too much depletion and the breakdown of the Gaussian theory, C_{nl} should then be as low as possible from a simulation point of view. From equation (A.8) we find, with $L_z = \alpha L^2 / (5N_0 a)$ implementing the 2D condition, for general parameters that

$$C_{nl} = \frac{1}{\alpha} \left(\frac{5N_0 a}{L} \right)^2. \quad (\text{A.12})$$

Since L is bounded from above by experimental constraints, the only way to realize low values of C_{nl} for a given atom number and fixed thickness is to reduce the scattering length. A lower particle number quadratically reduces the necessary value of C_{nl} .

In Bogoliubov theory, the quantum depletion is given in three dimensions by [Pitaevskii and Stringari, 2016]

$$\Delta = \frac{8N_0}{3\sqrt{\pi}} \sqrt{na^3} \propto (C_{nl})^{3/2}, \quad (\text{A.13})$$

implying that the parameter which controls the validity of Bogoliubov theory is

$$\frac{(C_{nl})^{3/2}}{N_0}. \quad (\text{A.14})$$

In two dimensions the depleted number of atoms can similarly be evaluated by a two dimensional integral over the squeezing occupation v_k^2 , which also converges at least for $T = 0$, and gives

$$\Delta \propto C_{nl}, \quad (\text{A.15})$$

implying that it is simply the ratio of

$$\frac{C_{nl}}{N_0} \quad (\text{A.16})$$

which controls the validity of the Bogoliubov theory.

Thus, we see for two dimensional condensates at $T = 0$, for getting to a regime where we understand the linearized theory and can apply TWA simulations easily, a low atom number is actually favorable, since the ratio C_{nl}/N_0 is proportional to N_0 in view of (A.12).

We conclude that a particle number of $N_0 = 10^4$, corresponding to an aspect ratio of the trap frequencies of $\gg 6.25$ for the above parameters (since the thickness can now be 10 times as much), and which would be a realistic set-up, is advantageous over $N_0 = 10^5$ particles also from a simulational point of view. We should then choose $C_{nl} \gg 6.25$, so for example $C_{nl} = 50$. For such low values of C_{nl} , however, time evolution is slow, and even the longest modes in the system are too short to be phononic. C_{nl} can be increased with scattering length, by a more flat condensate, or increasing the size of the system.

B. BECS Software Package

B.1. Installing and Running BECS

BECS has been successfully compiled under Linux and Mac with gcc 4.7.2 and under Windows with Visual Studio 2012.

B.1.1. Installing FFTW3

A main part of the computation time of the PGPE is spend with Fourier transforms. BECS makes use of the FFTW3 library (“Fastest Fourier Transform in the West”), which runs on the CPU. The FFTW3 library needs to be present to compile BECS.

The following is assuming you are on Linux/Mac. Two files are necessary:

- `fftw3.h` – A C “header file” with some definitions of functions of FFTW
- `libfftw3.a` (or similar) – a library that contains the actual machine code of FFTW

For performance reasons it is advisable to compile FFTW yourself on the machine on which BECS is going to run. Under Linux this is anyway the standard way to install any library. The following does not need root access.

1. Get the tar.gz file for fftw 3.3.4 or later from <http://www.fftw.org/download.html> and unpack
2. cd to the directory and type
 - a) `./configure --prefix=/home/.../some_temporary_dir --enable-sse2`

`--enable-avx` (the last two if you are on modern Intel CPU)

b) `make`

c) `make install`

3. If something goes wrong do

a) `make distclean`

b) and try again

4. For more information see

`http://www.fftw.org/fftw3\_doc/`
`Installation-on-Unix.html#Installation-on-Unix`

5. Create a folder for the BECS programme. Find

`some_temporary_dir/include/fftw3.h` and `some_temporary_dir/`
`lib/libfftw3.a`

and copy to the BECS folder.

B.1.2. Installing BECS

Simply copy the files `sim.py` (or `sim_win.py` under windows), `makefile`, `main.cpp`, `process.cpp` and `cfg.h` into the same directory which contains the 2 files from `fftw` from above. The Matlab file `ana3d.m` for analyzing the data can but does not need to be in this folder. Make sure the `#define WINDOWS` in `cfg.h` commented out under Linux and Mac and `#define MAC` is commented out under Linux and Windows (with `//`).

B.1.3. Running BECS

Make sure Python 3 is installed.

Edit `sim.py` and set `numthreads` to the number of physically available cores in your system (not taking into account the hyperthreading factor).

Edit `cfg.h` below line ≈ 60 to have the relevant parameters for the simulation you want to run (see comments there for more information) and `sim.py` to set the `save_dir` path, `save_prefix`, and `numtrajectories` for your simulation.

B.1.4. Running the simulation

You have multiple options: The standard one is to just run the python script, e.g. `python(3) sim.py &`

This script will do all of the following:

1. If necessary compiles BECS and process with make. This means it detects automatically if you have made changes to `cfg.h` recently and if so it will re-compile a highly optimized version of the BECS programme and the processing application for your set of parameters. Errors from compilation will be printed into the command line
2. Creates output folder for data
3. Creates joblist with `numtrajectories` jobs for becs simulation programme
4. Works through it in scheduled way having `numthreads` jobs running in parallel. The output from BECS is suppressed in the standard setting – see below how to switch it on.
5. It will automatically save a Matlab file named `options.m` to the save directory which contains all relevant options you have chosen in `cfg.h` and will be read in by the analysis script in Matlab, and is useful for future reference.
6. When all jobs are finished, calls process to process the data. The output from process is printed into the terminal.

In general, the usage is as follows: `python sim.py [numtrajectories] [-v]`

`Numtrajectories` option is optional and overwrites the value in the script. Iff it is used, `-v` option can be used to enter verbose mode, printing out the errors or progress / status that the becs programme would print into the terminal. It is expected that this is used mostly

for troubleshooting and test reasons when only one trajectory is run. Otherwise output gets messy anyway.

So a typical test run would be to

1. Change the number of steps in `cfg.h` to something small, e.g. 1000
2. call `python sim.py 1 -v`

Finally, you have the option of not using python at all and just calling `./becs` and `./process` yourself. Don't forget compiling it by calling `make`. Both applications expect the path to the save directory as a first argument. The directory must exist! As a second argument, BECS expects the ID of the current trajectory. Be sure that at least one call is with ID 0 because only the 0th trajectory saves the `options.m` file. `process` expects the number of trajectories as the second argument. E.g. for a single trajectory

1. Create a save directory, e.g. `/home/USER/becs/Data/`
2. `./becs /home/User/becs/Data 0`
3. Wait for it to finish
4. `./process /home/User/becs/Data 1`

In principle you can now delete all files apart from the `options.m` and the `ens_` files.

B.1.5. Analyzing the data

Make sure the path defined in the top of `ana3d.m` is set to the save directory and `process` has been run. Then just call `ana3d`. This file also works for 2D (it detects automatically which options you have chosen and does everything accordingly).

B.1.6. Summary

To sum up the typical workflow is to

1. Edit `cfg.h`

2. Set the save path in `sim.py`
3. execute `sim.py`
4. Set the same save path in the Matlab file `ana3d.m` and call it

You can even skip step 2 sometimes. Files will be overwritten if necessary.

C. Code

C.1. BECS core

We give the implementation of some of the algorithms developed to carry out TWA. The code is written in C and has been carefully optimized on a low level taking care of memory alignment issues and reusing buffers as much as possible instead of creating new variables to save processor cache space.

We only give the code for three dimensions. For two dimensions, the i -loops have to be dropped.

C.1.1. Initial sampling

In this code, it should be noted how an fftshift in Fourier space is avoided by alternating the sign in real space. Two quasiparticle excitations are sampled from the thermal Wigner function corresponding the $\pm\mathbf{k}$; the sum over real particles stops at the centre after going through half of the field, since the real particles for $-\mathbf{k}$ are already specified by those for $\mathbf{k}$. A generalised Bogoliubov transformation is used which accounts for the explicitly non-zero condensate phase (one could break the symmetry by hand initially, but at later points in time the condensate will obtain a phase, which beyond the linear theory will be nontrivially time-dependent). The sampling in Fourier space is only for the inner region (a box with half the side length centred on the condensate mode) which is not trivially projected out.

```
for (long i = 0; i < N; ++i)
{
```

```

    for (long j = 0; j < N; ++j)
    {
        for (long k = 0; k < N; ++k)
        {
            long index = i*N*N+j*N+k;
            dc_buff[index] = T(1.0)*DX*DX*DX;
            if ((i+j+k)%2==1)
                dc_buff[index]*=T(-1.0);
        }
    }
}

#ifdef LOW_PREC
    fftwf_execute(fftPlanForward);
#else
    fftw_execute(fftPlanForward);
#endif

long condensate_index = N/2*N*N+N/2*(N+1);
C_phase = std::exp(C(0,2*M_PI*myrandUni()));
dc_buff[condensate_index] *= phase;

for (long i = N/4; i <= N/2; ++i)
{
    for (long j = N/4; j <= 3*N/4; ++j)
    {
        for (long k = N/4; k <= 3*N/4; ++k)
        {
            if ( (i==N/2) && (j==N/2) && (k==N/2) )
                return;

            T_kx = (i-N/2)*DK;
            T_ky = (j-N/2)*DK;
            T_kz = (k-N/2)*DK;
            T_ksq = kx*kx+ky*ky+kz*kz;

```

```

T_omegak = sqrt(ksq/2*(ksq/2+2*
    ↪ Cnl(-1.0)));
T_vk = -sqrt((ksq/2 + Cnl(-1.0))
    ↪ /2/omegak - 0.5);
T_uk = +sqrt((ksq/2 + Cnl(-1.0))
    ↪ /2/omegak + 0.5);

C_b1 = C(0.0);
C_b2 = C(0.0);

if (WIGNER)
{
    T_nk = T(1.0)/(exp(
        ↪ omegak/(T0
        ↪ +0.0000001)) - T
        ↪ (1.0));
    //nk = T0/omegak;
    T_norm = sqrt(0.5+nk)/
        ↪ sqrt(2*N0);
    b1 = C(myrand()*norm,
        ↪ myrand()*norm);
    b2 = C(myrand()*norm, myrand()*
        ↪ norm);
}
else
{
    b1 = C(sqrt(T0/omegak/N0
        ↪ ));
    b2 = b1;
}

dc_buff[i*N*N+j*N+k] += phase*(
    ↪ uk*b1 + vk*std::conj(b2));
dc_buff[(N-i)*N*N+(N-j)*N+N-k]

```

```

                                ↪ += phase*(uk*b2 + vk*std::
                                ↪ conj(b1));
                                }
                                }
                                }

```

C.1.2. Maximally efficient RK4 implementation

```

inline void kernelPositionSpace(T * dpot, T C_nl)
{
    for (long i = 0; i < SIZE_FULL; ++i)
        dc_buff[i] = (dpot[i] + C_nl*(dc_buff[i].imag()*
            ↪ dc_buff[i].imag() + dc_buff[i].real()*
            ↪ dc_buff[i].real()))*dc_buff[i]/T(SIZE_FULL
            ↪ );
}

void F(T * pot, T t) {
    //in place ifft on dc_buff
#ifdef LOW_PREC
    fftwf_execute(fftPlanBackward);
#else
    fftw_execute(fftPlanBackward);
#endif
    T u = Cnl(t);
    kernelPositionSpace(pot, u);
#ifdef LOW_PREC
    fftwf_execute(fftPlanForward);
#else
    fftw_execute(fftPlanForward);
#endif
}

```

```

}

//this just multiplies with the exponentiated diagonal kinetic term in
  ↪ Fourier space saved in transform. The symmetry of the problem is
  ↪ exploited by reducing the size
//of the tranform buffer and indexing it properly
inline void trafo3D(C * dest, const C * transform) {
    //D=3: transform is only a  $(N/4+1)^3$  matrix (roughly 1/8 of
      ↪ projected region), this is sufficient!
    //only sum over projected region
    for (long i = N/4; i <= 3*N/4; ++i)
        for (long j = N/4; j <= 3*N/4; ++j)
            for (long k = N/4; k <= 3*N/4; ++k)
                {
                    long index = (N/4+1) * (N/4+1) * abs(i-N
                        ↪ /2) + (N/4+1) * abs(j-N/2) + abs(k
                        ↪ -N/2);
                    C fac = transform[index];
                    dest[i*N*N + j*N + k] *= fac;
                }
}

void subStep3D(C * dc, const C * dc_I, C * dc_buff, T a, T b, T timestep
  ↪ ) {
    //example for a=1/6, b=1/2: add buff/6 and c and save in c;
    //          add buff/2 and c_I and save in buff;

    projectionOuter3D();

    C ac = C(0.0, -timestep)*a;
    C bc = C(0.0, -timestep)*b;
    for (long i = N/4; i <= 3*N/4; ++i)

```

```

{
    for (long j = N/4; j <= 3*N/4; ++j)
    {
        for (long k = N/4; k <= 3*N/4; ++k)
        {
            long index = i*N*N + j*N + k;
            if (isOuter3D(i,j,k)) {
                dc_buff[index] = T(0.0);
                continue;
            }
            dc[index] += ac*dc_buff[index];
            dc_buff[index] = bc*dc_buff[index] +
                ↪ dc_I[index];
        }
    }
}

```

*//using the previous definitions, the core rk4 algorithm can then
 ↪ efficiently be expressed as*

```

trafo3D(dc, dtransform);
memcpy(dc_I, dc, SIZE_FULL * sizeof(C));
F(dc_buff, dpotential, t);
trafo3D(dc_buff, dtransform);
subStep3D(dc, dc_I, dc_buff, 1.0/6.0, 0.5, DELTA_T);
F(dc_buff, dpotential, t+DELTA_T/2);
subStep3D(dc, dc_I, dc_buff, 1.0/3.0, 0.5, DELTA_T);
F(dc_buff, dpotential, t+DELTA_T/2);
subStep3D(dc, dc_I, dc_buff, 1.0/3.0, 1.0, DELTA_T);
trafo3D(dc_buff, dtransform);
F(dc_buff, dpotential, t+DELTA_T);
trafo3D(dc, dtransform);
subStep3D(dc, dc_I, dc_buff, 1.0/6.0, 0.0, DELTA_T);

```

C. Code

```
t += DELTA_T;
```

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