

Chapter 1

Stochastic quantum dynamics in 1D and lattice systems

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We show that stochastic phase-space methods within the truncated Wigner approximation can be used to solve non-equilibrium dynamics of bosonic atoms in 1d traps. We consider systems both with and without an optical lattice and address different approximations in stochastic synthesis of quantum statistical correlations of the initial atomic field operator. We also present a numerically efficient projection method for analyzing correlation functions of the simulation results. Physical examples demonstrate non-equilibrium quantum dynamics of solitons and atom number squeezing in optical lattices in which case we, e.g., numerically track the soliton coordinates and calculate quantum mechanical expectation values and uncertainties for the position of the soliton.

1.1. Introduction

Atomic systems with enhanced quantum fluctuations can be prepared in tightly-confined cigar-shaped atom traps, where the strong transverse confinement suppresses density fluctuations along the radial direction of the trap (see, e.g., Ref. [1]). Quantum effects may be further strengthened by reducing the kinetic energy of the atoms by means of applying an optical lattice potential along the axial direction [2, 3]. In this article we describe the use of truncated Wigner approximation (TWA) [4–9] in dissipative non-equilibrium quantum dynamics of bosonic atoms in a 1d system both with and without an optical lattice. The TWA formalism can include

a very large number of degrees of freedom in the stochastic representation of the atomic field operator and dissipative dynamics emerges from a microscopic treatment of the unitary quantum evolution, due to energy dissipation within the large phase-space without any additional explicit damping terms in the Hamiltonian. Quantum and thermal fluctuations of the atoms may be included in the initial state and the resulting quantum statistical correlations of the initial state may be accurately synthesized for different quantum states in the Wigner representation. Some of the approaches presented in this article have been used in the studies of a fragmentation of a Bose-Einstein condensate (BEC) by turning-up of an optical lattice [7, 8], dissipative atom transport [10], dynamically unstable lattice dynamics [11], and dark solitons [12, 13].

We address different approximations in synthesization of quantum and thermal noise in the initial state. We start with a simple uniform system and phonon excitations within the Bogoliubov approximation. These are extended to non-uniform systems and situations where the back-action of the excited-state correlations on the ground-state atoms is included in self-consistent methods. A particular problem of analyzing non-equilibrium quantum dynamics in TWA, related to symmetric operator-ordering of the Wigner distributions is addressed by providing a numerically practical projection technique.

1.2. Methodology

1.2.1. Initial state generation in TWA

In the approach considered in the present case, 1d dynamics is unitary and quantum and thermal noise enter only through the stochastic initial state that generate the fluctuations of TWA dynamics. The dynamical evolution is governed by the Gross-Pitaevskii equation (GPE), but $\Psi_W(x, t)$ should be considered as a stochastic phase-space representation of the full field operator:

$$i\hbar \frac{\partial}{\partial t} \Psi_W = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V + g_{1d} N |\Psi_W|^2 \right) \Psi_W, \quad (1.1)$$

where the interaction strength $g_{1d} = 2\hbar\omega_{\perp}a$, the s -wave scattering length a , the total number of atoms N , and V is the trapping potential. Including noise only in the initial conditions is by no means necessary, however, since depending on the physical problem, we could include, e.g., atom losses via collisions and spontaneous emission that would generate also dynamical

noise terms for each time step. Since for the unitary evolution all the noise is incorporated in the initial state, it is especially important that the quantum mechanical correlation functions for the initial state of the atomic field operator are synthesized as accurately as practical for each particular physical problem. Here we follow the basic formalism of Refs. [7, 8] which has also been reviewed in [11] and further developed in [12, 13].

1.2.1.1. Uniform system

The simplest approach is a weakly interacting bosonic gas in a uniform space at $T = 0$ where we use the Bogoliubov approximation to model quantum fluctuations of the atoms. In the Bogoliubov theory we calculate the linearized fluctuations of the ground state (or a stationary GPE solution) in which case the back-action of the excited-state atoms on the ground state is ignored [14]. We write the decomposition

$$\hat{\Psi}(x) = \phi_0(x)\hat{\alpha}_0 + \hat{\psi}'(x), \quad (1.2)$$

where the total number of ground state atoms $N_c = \langle \hat{\alpha}_0^\dagger \hat{\alpha}_0 \rangle$. The fluctuation part $\hat{\psi}'$ for the excited states can be written in terms of quasi-particle operators $\hat{\alpha}_q$ and $\hat{\alpha}_q^\dagger$ as

$$\hat{\psi}'(x) = \frac{1}{\sqrt{L}} \sum_{q \neq 0} (u_q \hat{\alpha}_q e^{iqx - i\epsilon_q t} - v_q^* \hat{\alpha}_q^\dagger e^{-iqx + i\epsilon_q^* t}). \quad (1.3)$$

The normal mode frequencies ϵ_q and the quasi-particle amplitudes u_q and v_q can be solved straightforwardly and the expectation value of the number of excited-state atoms in the Bogoliubov theory is

$$\bar{N}' = \sum_q (|u_q|^2 + |v_q|^2) n_{\text{BE}}(\epsilon_q) + \sum_q |v_q|^2, \quad (1.4)$$

with $\langle \hat{\alpha}_q^\dagger \hat{\alpha}_q \rangle = n_{\text{BE}}(\epsilon_q) = [\exp(\epsilon_q/k_B T) - 1]^{-1}$ denoting the ideal Bose-Einstein distribution. At $T = 0$ we have $n_{\text{BE}}(\epsilon_q) = 0$.

In order to construct the initial state for the atoms in the TWA evolution we replace the quantum field operators ($\hat{\Psi}, \hat{\Psi}^\dagger$) by the classical fields (Ψ_W, Ψ_W^*) by using complex stochastic variables ($\alpha_q, \alpha_{q'}^*$) in the place of the quantum operators ($\hat{\alpha}_q, \hat{\alpha}_{q'}^\dagger$) in Eq. (1.3). In the Bogoliubov theory the operators ($\hat{\alpha}_q, \hat{\alpha}_q^\dagger$) form a set of ideal harmonic oscillators and at $T = 0$ ($\alpha_q, \alpha_{q'}^*$) are obtained by sampling the corresponding Wigner distribution function [15]

$$W(\alpha_q, \alpha_q^*) = \frac{2}{\pi} \exp[-2|\alpha_q|^2]. \quad (1.5)$$

In this case each unoccupied excitation mode is uncorrelated with Gaussian-distributed noise. The expectation value $\langle \alpha_q^* \alpha_q \rangle_W = \frac{1}{2}$ specifies the width of the distribution and represents vacuum noise, resulting from the symmetric ordering of the expectation values in the Wigner representation. The noise is distributed in space according to the plane waves, with a constant density. In the absence of any correlations between the modes, the vacuum noise in the uniform space could be replaced by uncorrelated Gaussian noise on evenly-spaced numerical grid points. However, the simplest modification to the Bogoliubov expansion is to fix the total atom number in each stochastic realization. This introduces long-wavelength correlations between the ground-state mode and the excited-state phonon modes, so that already in this simple example there exist non-trivial spatial noise correlations [12, 13]. For each stochastic realization the number of excited-state atoms satisfies

$$N' = \sum_q (|u_q|^2 + |v_q|^2) (\alpha_q^* \alpha_q - \frac{1}{2}) + \sum_q |v_q|^2. \quad (1.6)$$

with the ensemble average $\bar{N}' = \sum_q |v_q|^2$. In Eq. (1.6) we have transformed the symmetric ordering of the Wigner representation to quantum expectation values of normally-ordered operators by subtracting $\langle \alpha_q^* \alpha_q \rangle_W = \frac{1}{2}$ from each mode. The ground-state atom number is then obtained from the fixed total atom number N , so that in each stochastic realization $N_c = N - N'$ and we set $\alpha_0 = \sqrt{N_c + 1/2}$. The ensemble average of the ground-state population $\bar{N}_c = N - \bar{N}'$.

At $T \neq 0$ we replace Eq. (1.5) by [15]

$$W(\alpha_q, \alpha_q^*) = \frac{2}{\pi} \tanh(\xi_q) \exp[-2|\alpha_q|^2 \tanh(\xi_q)], \quad (1.7)$$

where $\xi_q \equiv \epsilon_q/2k_B T$. The Wigner function is Gaussian-distributed with the width $n_{\text{BE}}(\epsilon_q) + 1/2$. The formula introduces thermal populations of each quasi-particle mode and generates more complex spatial noise correlations. After the noise generation, the initial state for stochastic evolution may be written as

$$\Psi_W(x, 0) = \phi_0(x) \alpha_0 + \frac{1}{\sqrt{L}} \sum_{q \neq 0} (u_q \alpha_q e^{iqx} - v_q^* \alpha_q^* e^{-iqx}). \quad (1.8)$$

Here $\Psi_W(x, 0)$ is a stochastic representation of the full field operator for the atoms.

1.2.1.2. Trapped gases

In a harmonic trap, or in a combined harmonic trap and optical lattice, the atoms experience a non-uniform potential that introduces spatially-varying initial noise distribution even at $T = 0$. We write the external potential as $V(x) = m\omega^2 x^2/2 + sE_R \sin^2(\pi x/d)$, where $E_R = \hbar^2 \pi^2/2md^2$ is the lattice photon recoil energy and d is the lattice period. The Bogoliubov equations now become spatially dependent and need to be solved numerically [14]. In Eq. (1.3) we replace $u_q e^{iqx}/\sqrt{L} \rightarrow u_j(x)$ and $v_q e^{iqx}/\sqrt{L} \rightarrow v_j(x)$ where the index j refers to the mode number. In the lowest order approximation the quasi-particle mode functions $u_j(x)$ and $v_j(x)$ are obtained in the Bogoliubov theory. In several cases of interest where the multi-mode structure of the excitations become important, the Bogoliubov approximation is insufficient due to large contribution of the quadratic fluctuation terms, and one consequently needs to use a higher-order theory, such as the gapless Hartree-Fock-Bogoliubov (HFB) formalism in which case the ground-state and the excited-state populations are solved self-consistently. The coupled HFB equations for the ground state and excitations read [16, 17]

$$\left(\hat{\mathcal{L}} - U_c \bar{N}_c |\phi_0|^2 \right) \phi_0 = 0 \quad (1.9)$$

$$\begin{aligned} \hat{\mathcal{L}} u_j - U_c \bar{N}_c \phi_0^2 v_j &= \epsilon_j u_j, \\ \hat{\mathcal{L}} v_j - U_c \bar{N}_c \phi_0^{*2} u_j &= -\epsilon_j v_j. \end{aligned} \quad (1.10)$$

where $u_j(x)$ and $v_j(x)$ ($j > 0$) are restricted to the subspace orthogonal to ϕ_0 . Here

$$\hat{\mathcal{L}} \equiv -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) + 2U_c \bar{N}_c |\phi_0|^2 + 2U_e n'(x) - \mu \quad (1.11)$$

and μ is the chemical potential. In Eq. (1.10) the Bogoliubov approximation is obtained by setting $U_c = g_{1d}$, $U_e = 0$. In the gapless HFB theory (the G1 version in Ref. [17]), $U_c = g_{1d} [1 + m'(x)/\bar{N}_c \phi_0^2]$ and $U_e = g_{1d}$; here, the depleted density $n'(x) = \langle \hat{\psi}^\dagger(x) \hat{\psi}'(x) \rangle$, and the anomalous pair correlation $m'(x) = \langle \hat{\psi}'(x) \hat{\psi}'(x) \rangle$ introduce back-action of the excitations on the ground-state such that Eqs. (1.9) and (1.10) must be solved iteratively until the solutions converge. In the non-uniform case the number of excited-state atoms is given by

$$\bar{N}' = \int dx \sum_j [n_{\text{BE}}(\epsilon_j) (|u_j(x)|^2 + |v_j(x)|^2) + |v_j(x)|^2], \quad (1.12)$$

and the total atom number may be fixed in each realization as in the uniform case [12, 13].

1.2.1.3. Quasi-condensate description

In tightly-confined 1d traps, the phase fluctuations may be enhanced compared to those obtained using the standard Bogoliubov theory. A more accurate description can be calculated using quasi-condensate formalism that can be particularly important, e.g., to phase kinks [12, 13]. In the quasi-condensate description we write the field operator as [18]

$$\hat{\Psi}(x, 0) = \sqrt{n_0(x) + \delta\hat{n}(x)} \exp(i\hat{\theta}(x)). \quad (1.13)$$

The density $\delta\hat{n}(x)$ and phase $\hat{\theta}(x)$ operators may be written in the Bogoliubov-type expansion, requiring $\delta\hat{n}/n_0$ and $|\delta l \Delta \hat{\theta}|$ to be much less than one, where δl is the spacing on the numerical grid on which we calculate the operators and $\Delta \hat{\theta}$ is the gradient of the phase operator across one gridpoint. Thus (for $j > 0$)

$$\hat{\theta}(x) = \frac{-i}{2\sqrt{n_0(x)}} \sum_j \left(\theta_j(x) \hat{\alpha}_j - \theta_j^*(x) \hat{\alpha}_j^\dagger \right), \quad (1.14)$$

$$\delta\hat{n}(x) = \sqrt{n_0(x)} \sum_j \left(\delta n_j(x) \hat{\alpha}_j + \delta n_j^*(x) \hat{\alpha}_j^\dagger \right), \quad (1.15)$$

where $\theta_j(x) = u_j(x) + v_j(x)$ and $\delta n_j(x) = u_j(x) - v_j(x)$ are given in terms of the solutions to the Bogoliubov equations (see the previous section). This results in a stochastic Wigner representation $(\theta_W(x), \delta n_W(x))$ of phase and density operators. The stochastic initial state for the time evolution then reads [12, 13]

$$\Psi_W(x, 0) = \sqrt{n_{0,W}(x) + \delta n_W(x)} \exp(i\theta_W(x)), \quad (1.16)$$

where the ground-state density $n_{0,W}(x) = (N_c + 1/2)|\phi_0(x)|^2$.

1.2.1.4. Relaxation

We may also consider an ideal, non-interacting BEC as an initial state for the TWA simulations, but before the actual time evolution, we can continuously turn up the nonlinear interactions between the atoms. If the process is slow enough and relaxes to the ground state, we may be able to produce the stochastic initial state of the interacting system. Although this may simplify the calculations, in practise the technique in a closed system does not necessarily converge to the correct interacting state [8]. More complex models with open systems, kinetic equations and time-dependent noise can help the relaxation process at finite temperatures [19].

1.2.2. Wigner representation and symmetric ordering

The Wigner distribution returns symmetrically-ordered expectation values of any stochastic representations of quantum operators. In particular, the expectation values of the full multi-mode Wigner fields in the TWA simulations of the time-dynamics are symmetrically ordered with respect to every mode. In general, this can significantly complicate the analysis of the numerical results when quantum fluctuations are important [8]. A numerically practical transformation of the symmetrically-ordered expectation values to the normally-ordered expectation values of physical observables can be done using projection techniques (as shown Refs. [7, 8]). In the presence of an optical lattice, a natural approach is to project the stochastic field to the several lowest mode functions of the individual lattice sites. We define the amplitude of the i th mode of the site j as

$$a_{i,j}(t) = \int_{j^{\text{th well}}} dx [\varphi_j^{(i)}(x, t)]^* \Psi_W(x, t), \quad (1.17)$$

where Ψ_W is the stochastic field and $\varphi_j^{(i)}$ is the i th mode function of the well j . The integration is performed over the j th site and the site population reads

$$\langle \hat{n}_j \rangle = \sum_i \langle \hat{a}_{i,j}^\dagger \hat{a}_{i,j} \rangle = \sum_i [\langle a_{i,j}^* a_{i,j} \rangle_W - 1/2] \quad (1.18)$$

where $\langle \dots \rangle$ denotes the normally ordered expectation value of the quantum operators, and $\langle \dots \rangle_W$ the symmetrically-ordered expectation values obtained from the TWA simulations. Fluctuations are calculated using analogous transformations. For the on-site fluctuations of the atom number in the j th site we obtain

$$\begin{aligned} (\Delta n_j)^2 &= \langle \hat{n}_j^2 \rangle - \langle \hat{n}_j \rangle^2 \\ &= \sum_{i,k} [\langle a_{i,j}^* a_{i,j} a_{k,j}^* a_{k,j} \rangle_W - \langle a_{i,j}^* a_{i,j} \rangle_W \langle a_{k,j}^* a_{k,j} \rangle_W - \delta_{ik}/4]. \end{aligned} \quad (1.19)$$

Similarly, the relative atom number fluctuations between the sites p and q are obtained from

$$\begin{aligned} [\Delta(\hat{n}_p - \hat{n}_q)]^2 &= \sum_{i,k} [\langle (a_{i,p}^* a_{i,p} - a_{i,q}^* a_{i,q}) (a_{k,p}^* a_{k,p} - a_{k,q}^* a_{k,q}) \rangle_W \\ &\quad - \langle a_{i,p}^* a_{i,p} - a_{i,q}^* a_{i,q} \rangle_W \langle a_{k,p}^* a_{k,p} - a_{k,q}^* a_{k,q} \rangle_W - \delta_{ik}/2]. \end{aligned} \quad (1.20)$$

Alternatively, we could have, for instance, written

$$\begin{aligned} \langle \hat{n}_j \rangle &= \int_j dx \langle \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \rangle = \int_j dx \langle \Psi^*(x) \Psi(x) \rangle_W \\ &\quad - \frac{1}{2} \int_j dx \sum_i (|u_i(x)|^2 - |v_i(x)|^2). \end{aligned} \quad (1.21)$$

Calculation of $\langle \hat{n}_j^2 \rangle$ then, however, results in double integrals over the sites that can be computationally slow when performed over a large number of realizations.

1.3. Applications

1.3.1. Dark solitons

Dark solitons have been actively studied in BECs and in nonlinear optics. Although there exist numerous studies of classical solitons, the quantum properties of dark solitons are much less known. Numerical TWA simulations are suitable for the studies of the creation and non-equilibrium quantum dynamics of solitons in 1d traps. We consider the experimental imprinting method [20, 21], where a soliton is generated by applying a ‘light-sheet potential’, of value V_ϕ to half of the atom cloud, for time τ , so that in the corresponding classical case the light sheet imprints a phase jump of $\phi_c = V_\phi \tau / \hbar$ at $x = 0$, preparing a dark soliton. Classically the imprinted soliton oscillates in a harmonic trap at the frequency $\omega / \sqrt{2}$ [22] with the initial velocity $\mathbf{v}/c = \cos(\phi_c/2)$, depending on ϕ_c and the speed of sound c . The soliton is stationary (dark) for $\phi_c = \pi$, with a zero density at the kink. Other phase jumps produce moving (grey) solitons, with non-vanishing densities at the phase kink.

In TWA simulations we generate the initial state using the quasi-condensate formalism and vary the ground-state depletion \bar{N}'/N . At $T = 0$ we keep the nonlinearity Ng_{1d} fixed, but adjust the ratio g_{1d}/N . This is tantamount to varying the effective interaction strength $\gamma_{\text{int}} = mg_{1d}/\hbar^2 n$. We can also study the effects of thermal depletion by varying T .

In quantum case, soliton trajectories in TWA fluctuate between different realizations. Individual stochastic realizations of $|\Psi_W|^2$ in a harmonic trap represent possible experimental observations of single runs. In TWA we can ensemble average hundreds of stochastic realizations in order to obtain quantum statistical correlations of the soliton dynamics. We numerically track the position of the kink at different times in individual realizations

and calculate the quantum mechanical expectation values for the soliton position $\langle \hat{x} \rangle$ and its uncertainty $\delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2}$.

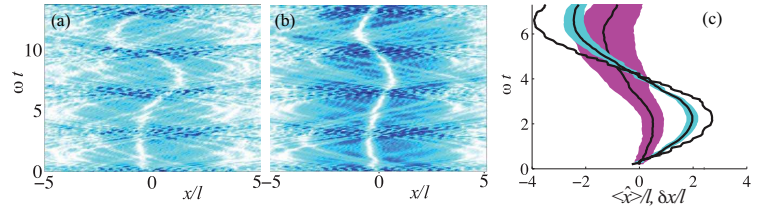


Fig. 1.1. Soliton dynamics in a harmonic trap showing (a-b) the Wigner density $|\Psi_w(x, t)|^2$ for individual stochastic realizations with the same $g_{1d}N = 100\hbar\omega l$, $\phi_c = 2$, and $T = 0$ for $N = 50, 100$, in (a) and (b), respectively; (c) The quantum mechanical expectation value for the soliton position $\langle \hat{x} \rangle$ (solid lines) and its uncertainty δx (shaded regions) for $N = 8000, 440, 50$ (curves with decreasing amplitudes) with the same non-linearity $g_{1d}N$, $\phi_c = 2$, and $T = 0$. At $N \simeq 8000$, δx is negligible. Quantum fluctuations increase δx and soliton damping, and decrease the speed.

1.3.2. Atom number squeezing

In this section we consider an example of a TWA calculation of atom number squeezing due to turning up of an optical lattice. Unlike in Refs. [7, 8] where a BEC fragmentation in TWA was investigated by a lattice with a large number of small sites, we simulate a six-site system with considerable multi-mode effects within individual sites. Bose-condensed ^{87}Rb atoms are confined to a cigar-shaped optical dipole trap where an optical lattice is applied along the axial direction [23]. The lattice potential is slowly turned up from $s(0) = 48E_R$ to $s(\tau) = 96E_R$. The harmonic trap frequency is $\omega = 2\pi \times 21\text{Hz}$, the atom number $N \simeq 5000$, and the lattice spacing $d \simeq 5.7\mu\text{m}$. The system was also realized in the recent atom number fluctuation experiment [24].

Due to large individual lattice sites the multi-mode structure of the fluctuations is important, and the atom number fluctuations are evaluated by using the projection technique to several modes in each site, as explained in the previous section. The Bogoliubov approximation is not accurate due to phonon-phonon interactions and the initial state is calculated using the HFB method. The spatially non-uniform distribution of quantum and thermal fluctuations is clearly seen in Fig. 1.2. The lowest HFB modes dominantly occupy the outer regions of the atom cloud with significantly enhanced atom number and phase fluctuations in those sites. Such fluctua-

tions could not be represented, e.g., by a uniform stochastic noise sampling.

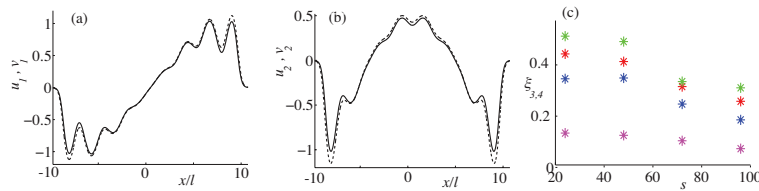


Fig. 1.2. The numerical solution of the lowest two HFB modes in a six-site optical lattice showing (a) $u_1(x)$ (dotted) and $v_1(x)$ (solid); (b) $u_2(x)$ (dotted) and $v_2(x)$ (solid) at $s = 24$ and $T \simeq 5.5$ nK; (c) Relative atom number squeezing at different lattice height between two central nearest-neighbor sites $\xi_{pq} = [\Delta(\hat{n}_p - \hat{n}_q)]^2 (n_p + n_q) / (4n_p n_q)$. The different data sets correspond to temperatures (from top to bottom) $T \simeq 5.5$ nK, $T \simeq 4.5$ nK, $T \simeq 4.0$ nK, and $T = 0$.

1.4. Comparisons

Generating quantum noise in TWA in 2d and 3d may have problems in terms of heating the atom cloud during time evolution due to rapid coupling dynamics between the modes [6] and divergence of physical observables as a function of the number of modes, but 1d systems have been more robust. Although clearly insufficient, e.g., in a Mott-insulator regime and at very low atom numbers, TWA has been successful in describing superfluid dynamics in the presence of considerable quantum fluctuations. For instance, TWA simulations [10] were qualitatively able to produce the experimentally observed damping rate of center-of-mass oscillations of bosonic atomic cloud in a very shallow, strongly confined 1D optical lattice, corresponding to the dissipative atom transport experiments of Ref. [2].

The accuracy of the initial state noise generation can be a crucial limitation, especially in simulations involving very short time dynamics. The spatial distribution of phonon excitations in trapped systems can result in very rapid noise variation where, e.g., phase fluctuations are dominated close to the edges of the atom cloud [8]. For dark soliton dynamics, the differences in the soliton trajectories between the cases in which the noise was generated within the quasi-condensate description and in the Bogoliubov theory are notable [12]. Evaluating phonon modes in the linearized Bogoliubov approximation may also become inaccurate, compared to self-consistent HFB methods.

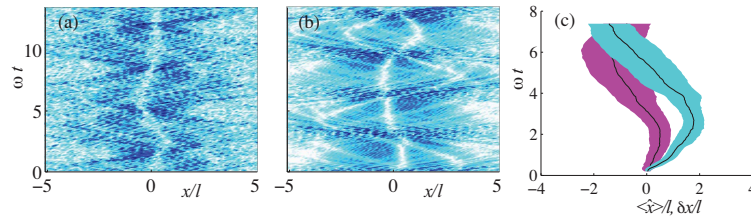


Fig. 1.3. Differences between initial noise generation in TWA. Dark soliton dynamics in a 1d harmonic trap showing (a-b) the Wigner density $|\Psi_w(x, t)|^2$ for individual stochastic realizations of TWA for $\phi_c = 2$, $T = 0$, and $N = 50$ (parameters as explained in 1.3.1). In (a) the initial state is generated within the Bogoliubov approximation and in (b) using the quasi-condensate formalism; (c) The quantum mechanical expectation values for the soliton position $\langle \hat{x} \rangle$ (solid lines) and its uncertainty δx (shaded regions). The lighter curve with larger oscillation amplitude corresponds to the Bogoliubov case and the darker one the quasi-condensate case.

Acknowledgments

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