Chapter 1

Number-Conserving Stochastic Approaches for Equilibrium and Time-Dependent Bose Gases

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We review several number-conserving stochastic field methods for equilibrium and time dependent Bose gases; these range from classical field to exact methods, and include truncated Wigner (with an explicitly number-conserving implementation), and, only for equilibrium, a semiclassical field method. Stochastic elements in the initial state mimic thermal fluctuations in the classical field, or thermal and quantum fluctuations in the Wigner, semiclassical and exact methods. Time evolution is deterministic with the nonlinear Schrödinger equation for the classical field and Wigner methods while it is stochastic for the exact method. We illustrate each method by relevant applications to the physics of quantum gases.

1.1. Introduction

In classical physics we can study the dynamics and equilibrium properties of a system with the phase space probability density. The closest quantum equivalents to this are the quasi-probability distributions widely used in quantum optics. Two important examples are the Wigner distribution and the Glauber-P distribution. Unfortunately their evolution equations are not always possible to implement in practice in an exact way because they involve terms that are not simply mappable to a classical deterministic or stochastic process, such as diffusive terms with a non-positive diffusion tensor or terms involving cubic derivatives of the distribution function. One is then led naturally to approximate them in different

ways, each of which has its strengths and weaknesses, and might or might not be adapted to the particular physical situation. In this chapter we describe several such approaches for equilibrium and non-equilibrium Bose systems (see also Chapters **??**, **??** - **??**, **??**). The first approach is based on the Wigner distribution. The others are based on the Glauber-P distribution or its extensions, presenting different degrees of approximation: from the simplest classical field approach to exact methods. The methodology is quite similar for all the approaches and the unifying thread is that they are based on theories with a fixed total number of particles (also called "number conserving"). In other words the $U(1)$ symmetry is not broken. Number conservation can be important in some physical situations, for example the coherence time of a condensate depends crucially on fluctuations in the number of particles [1, 2]. From a formal point of view the approaches allow for a detailed quantitative comparison with perturbative theories in order to understand their limits of validity, such as with the Bogoliubov number conserving theory [3, 4] (see also Chapter **??**). We now give a very short description of each method.

The *Wigner method* allows us to include not only thermal but also quantum fluctuations [5–7] that are important to describe spontaneous processes [8], quantum dynamics, squeezing [9–11], etc. (see also Chapter **??**). For a system in equilibrium, the method we present is equivalent to the number conserving Bogoliubov theory of [4] valid for low enough non-condensed fraction. The real-time evolution is approximated (truncated Wigner) which leads to the principal limitations of this method. Indeed the thermal equilibrium state is not stationary under the approximated real time evolution and tends to thermalise to a classical distribution at a higher temperature. The method can nevertheless be very useful either (i) in the perturbative regime where it allows for a simple implementation of the time-dependent Bogoliubov number conserving approach or (ii) beyond the perturbative regime to include all the nonlinear processes, provided that the thermalization timescale is longer than the one of interest. This is more often the case in one dimension where the thermalization times are long (for related treatments in one-dimensional systems see Chapters **??**, **??** and **??**). In three spatial dimensions, for an ergodic system, the thermalization to a classical distribution may in some cases be too fast for the Wigner approach to be useful.

If one is mainly interested in thermal fluctuations and multimode effects, it might therefore be preferable to give up quantum fluctuations from the beginning and sample directly a classical field distribution that is stationary under real time evolution. This is the *classical field* model (see also Chapters **??**, **??** and **??**) which can be solved exactly on a computer. From our viewpoint it is thus very useful to test some analytical approximations e.g. perturbative or linearized ap-

proaches as in [1, 2]. Its main problem is that it is a classical model while reality is quantum. Furthermore it requires an energy cut-off and the results are *in general* cut-off dependent (for a discussion of possible ways of dealing with the cut-off see Chapters **??**, **??** and **??**). It is useful when the interesting physics is given by low-energy highly populated modes [12–14] which requires in practice $k_B T > \mu$ for an interacting system. Among its successes, the classical field model has been used to study the formation dynamics of a condensate [15, 16], to study phase coherence in Bose-Einstein condensates [1, 2], to get quantitative predictions for the transition temperature in 3d and in 2d thanks to a clever solution to the cut-off dependence issue [17–19], to study thermal vortices in a 2d Bose gas [20], to study analytically correlation functions in 1d [21], and to study the formation of solitons during evaporative cooling via the Kibble-Zurek mechanism [22].

When restricted to thermal equilibrium, the cut-off dependence can be eliminated by constructing a *semiclassical field theory* [23] which is intermediate between the full quantum theory and the classical field model. It is exact for the ideal gas. For the interacting gas it becomes increasingly accurate as the temperature increases. It smoothly interpolates between a classical description of the low-energy modes and the Bose-Einstein distribution for the weakly interacting high-energy modes. We have also developed *exact schemes* both for equilibrium [24] and non-equilibrium [25] systems. Unlike other exact methods e.g. path integral Monte Carlo [26–28] they do not privilege position space observables. Their limitation is that the computational effort grows exponentially with the system size.

1.2. Methodology

For all the methods in this chapter, we start with the same model Hamiltonian, where position space is discretized on a cubic grid with lattice constant b, with periodic boundary conditions of period $L_\nu = n_\nu b$ along direction $\nu = x, y, z$, and n_ν even integer (for definiteness, here we discuss the 3d case). We denote $\mathcal{N} \equiv \prod_\nu n_\nu$ the number of points on the grid, $V \equiv \prod_\nu L_\nu$ the quantization volume and $dV \equiv b^3$ the volume of the grid unit cell. In the case of a trapped gas, the quantization volume is large enough so that the atomic density is small near the boundaries. The Hamiltonian reads

$$\hat{H} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} + dV \sum_{\mathbf{r}} V_{\rm ext}(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) + \frac{g_0}{2} dV \sum_{\mathbf{r}} \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \,. \tag{1.1}$$

The field operator obeys the discrete bosonic commutation relations $[\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r}')] = (1/dV)\delta_{\mathbf{r},\mathbf{r}'}$, where the single-particle operator $\hat{a}_{\mathbf{k}}$ annihilates a particle of momentum $\mathbf{k}$, with $k_\nu \in (2\pi/L_\nu)\{-n_\nu/2, \ldots, n_\nu/2 - 1\}$. The successive

terms in (1.1) represent the kinetic energy, the trapping potential energy, and the atomic interactions modeled by a purely on-site interaction, with a bare coupling constant g_0 related to the effective coupling constant $g = 4\pi\hbar^2 a/m$ (where a is the s-wave scattering length - see Chapter **??**) by

$$\frac{1}{g} = \frac{1}{g_0} + \int_{[-\pi/b,\pi/b]^3} \frac{d^3k}{(2\pi)^3} \frac{m}{\hbar^2 k^2} \ . \tag{1.2}$$

To recover the continuous space physics, b is taken to be smaller than both the healing length ξ and the thermal de Broglie wavelength λ. In the degenerate and weakly interacting regime, $|a| \ll \xi, \lambda$, one can further take $b \gg |a|$ so that $g_0 \simeq g$ [29, 30]. In the approximate methods (Secs. 1.2.1, 1.2.2), we neglect the difference between g_0 and g, while g_0 is kept in H in the exact method (Sec. 1.2.3).

1.2.1. *Number-Conserving Wigner Method*

As is well known in quantum optics [31], the Wigner quasi-probability distribution $W(\Phi)$ of the complex classical field $\Phi(\mathbf{r})$ is a representation of the system density operator, such that its moments give the totally symmetrized expectation values of the quantum field $\hat{\Psi}$. For example, for the mean density $\rho(\mathbf{r})$ in $\mathbf{r}$, one has $\langle \Phi^*(\mathbf{r})\Phi(\mathbf{r})\rangle_e = \frac{1}{2}\langle \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}) + \hat{\Psi}(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\rangle = \rho(\mathbf{r}) + 1/(2dV)$. It is generally expected that the classical field approximation, that consists in replacing field operators by complex fields in the equations of motion, is the most accurate within the Wigner representation. For the simple case of an interacting thermal mode with initial large thermal occupation $\bar{n}$, the usual argument is that, in the equation of motion for the Wigner distribution, the classical field approximation amounts to neglecting terms that are cubic derivatives of W rather than quadratic for Glauber-P or Husimi-Q, wich is a factor $1/\bar{n}$ smaller approximation [32]. Furthermore, W remains positive for states with interesting quantum correlations, such as squeezed states of the field, whereas e.g. the Glauber P distribution is then singular.

Sampling of W at thermal equilibrium: In general, W is not positive for all Φ for non-Gaussian states of the field. Here we are restricted to an approximate sampling in the Bogoliubov approximation (see also Chapters **??**, **??**), for a temperature T much smaller than the critical temperature and for the weakly interacting regime. A further approximation is introduced in the sampling of the component of Φ on the condensate mode, valid when a large number of modes are thermally populated (e.g. $k_B T \gg \hbar\omega$ in a harmonic trap), that enforces the positivity of the

Wigner distribution. Finally, the field is written as

$$\Phi(\mathbf{r}) = e^{i\theta}\left[\sqrt{N_c}\left(\phi(\mathbf{r}) + \frac{\phi_\perp^{(2)}(\mathbf{r})}{N}\right) + \Lambda(\mathbf{r})\right], \tag{1.3}$$

where ϕ solves the time-independent Gross-Pitaevskii equation $H_{\rm GP}\phi \equiv \left[\frac{p^2}{2m} + V_{\rm ext}(r, t=0) + Ng|\phi|^2 - \mu_{\rm GP}\right]\phi = 0$, the chemical potential in the Gross-Pitaevskii approximation is denoted by $\mu_{\rm GP}$ and $\phi_\perp^{(2)}$ is the first correction to the condensate wavefunction beyond Gross-Pitaevskii and is orthogonal to ϕ. The equation for $\phi_\perp^{(2)}$ is given in [4]. The phase θ is chosen uniformly in the interval $[0, 2\pi]$. The non-condensed field Λ is orthogonal to ϕ. It is generated according to the Gaussian probability distribution

$$P(\Lambda, \Lambda^*) \propto \exp\left\{-dV(\Lambda^*, \Lambda)\cdot M \begin{pmatrix} \Lambda \\ \Lambda^* \end{pmatrix}\right\} \tag{1.4}$$

where $M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\tanh\left(\mathcal{L}/2k_BT\right)$ is expressed in terms of

$$\mathcal{L} = \begin{pmatrix} H_{\rm GP} + NgQ_\phi|\phi|^2Q_\phi & NgQ_\phi\phi^2Q_\phi^* \\ -NgQ_\phi^*\phi^{*2}Q_\phi & -H_{\rm GP}^* - NgQ_\phi^*|\phi|^2Q_\phi^* \end{pmatrix}. \tag{1.5}$$

Here the $2\mathcal{N}\times 2\mathcal{N}$ matrix $\mathcal{L}$ is the discretised version of the number conserving Bogoliubov operator and the $\mathcal{N}\times\mathcal{N}$ matrix Q_ϕ projects orthogonally to the condensate wavefunction ϕ, $(Q_\phi)_{\mathbf{rr}'} = \delta_{\mathbf{rr}'} - dV\phi(\mathbf{r})\phi^*(\mathbf{r}')$. We developed methods to sample (1.4) based on a Brownian motion of Λ [29, 33]. If the eigenvectors (u_k, v_k) of $\mathcal{L}$ with eigenvalues ϵ_k are known, we can directly use the modal expansion $\Lambda(\mathbf{r}) = \sum_k[\alpha_k u_k(\mathbf{r}) + \alpha_k^* v_k^*(\mathbf{r})]$ and sample the probability distribution of the complex amplitude α_k,

$$P_k(\alpha_k) = \frac{2}{\pi}\tanh\left(\frac{\epsilon_k}{2k_BT}\right)\exp\left[-2|\alpha_k|^2\tanh\left(\frac{\epsilon_k}{2k_BT}\right)\right]. \tag{1.6}$$

Finally, the condensate atom number N_c in (1.3) is expressed in terms of the non-condensed field Λ as

$$N_c = C - \frac{1}{2}dV(\Lambda^*, \Lambda)\cdot\left[\mathrm{Id} - M^2\right]\begin{pmatrix}\Lambda \\ \Lambda^*\end{pmatrix}, \tag{1.7}$$

where $C = N - \frac{1}{4}\mathrm{Tr}\,M + \frac{1}{2}(\mathcal{N}-1)$ and $\mathcal{N}$ the number of points on the grid.

Time evolution: Once a stochastic field Φ is generated, one evolves it deterministically with the usual time dependent Gross-Pitaevskii equation,

$$i\hbar\frac{\partial\Phi(\mathbf{r}, t)}{\partial t} = \left(\frac{p^2}{2m} + V_{\rm ext}(\mathbf{r}, t) + g|\Phi(\mathbf{r}, t)|^2\right)\Phi. \tag{1.8}$$

This corresponds to the truncated Wigner approximation, where cubic derivatives of W with respect to Φ or Φ^* are neglected in the exact equation of motion of W. Expectation values of (symetrically ordered) observables are obtained by averaging over many independent realisations of Φ. As mentioned in the introduction, the initial Wigner distribution is not stationary for the approximate evolution (1.8). This can be a limitation of the method especially in ergodic systems [29].

1.2.2. *Giving Up Quantum Fluctuations: A Classical Field Model*

The classical field model is defined by a Hamiltonian H which is formally identical to Eq. (1.1) but for a classical field, so that one has to change $\hat{\Psi} \to \Phi$ and $\hat{\Psi}^\dagger \to \Phi^*$. The Poisson brackets are $i\hbar\{\Phi(\mathbf{r_1}), \Phi^*(\mathbf{r_2})\} = \frac{\delta_{\mathbf{r}_1,\mathbf{r}_2}}{dV}$ so that $df/dt = \{f, H\}$ for a time-independent functional f of the field Φ.

Generation of the fields in the canonical ensemble: The classical fields are generated by sampling the classical distribution $P_{\rm cl}(\Phi) = \delta\left(\|\Phi\|^2 - N\right) e^{-\beta H}/Z$ where H is the classical Hamiltonian, Z a normalisation factor and $\|\Phi\|^2 \equiv \sum_{\mathbf{r}} dV|\Phi(\mathbf{r})|^2$. The approximate sampling scheme that we described for the Wigner method in the Bogoliubov limit is readily adapted to the classical field case as follows: one still uses Eq. (1.3), Λ is obtained from the probability distribution (1.4) by linearizing the hyperbolic tangent appearing in the matrix M, and N_c is adjusted to have $\|\Phi\|^2 = N$.

Moreover, contrarily to the Wigner quasi-distribution, $P_{\rm cl}$ is always positive and can be sampled exactly using well developed classical methods. For example, a Brownian motion simulation scheme (see p. 125 in [34]) consists in evolving Φ in the long imaginary time limit $\tau \to +\infty$ with the Ito stochastic process

$$d\Phi = -\frac{d\tau}{2} Q_\Phi H_{\rm NSLE}\Phi + \left(\frac{k_B T}{dV}\right)^{1/2} Q_\Phi dW - \left(\frac{\mathcal{N}-1}{2N}\right) k_B T d\tau \Phi \qquad (1.9)$$

where $H_{\rm NSLE} = \frac{p^2}{2m} + V_{\rm ext}(r, t=0) + g|\Phi|^2$, Q_Φ projects orthogonally to Φ and $dW(\mathbf{r})$ is a Gaussian noise with zero mean and a covariance matrix $\langle dW(\mathbf{r}) dW(\mathbf{r}')\rangle = 0$ and $\langle dW(\mathbf{r}) dW^*(\mathbf{r}')\rangle = \delta_{\mathbf{r},\mathbf{r}'} d\tau$.

Time evolution : Each of the generated fields is then evolved in real time with Eq. (1.8), which is exact within the classical field model.

1.2.3. *Exact and Semiclassical Methods*

One can show that the thermal equilibrium density operator in the canonical ensemble may be written as a stochastic average of dyadics of the form $\rho = \langle |N:\Phi_1\rangle\langle N:\Phi_2|\rangle_{\rm stoch}$, where $|N:\Phi\rangle$ is a Fock state with N particles in the non-necessarily normalized state Φ. The distribution of the $\Phi_{\alpha=\{1,2\}}$ is sampled by the

Ito stochastic process for $\tau = 0 \to \beta = 1/k_B T$:

$$d\Phi_\alpha(\mathbf{r}) = -\frac{d\tau}{2}\left[\frac{p^2}{2m} + V_{\rm ext}(\mathbf{r}, t=0) + g_0\left(\frac{N-1}{\|\Phi_\alpha\|^2}\right)|\Phi_\alpha(\mathbf{r})|^2 - g_0\left(\frac{N-1}{2}\right)\frac{\sum_{\mathbf{r}'} dV\,|\Phi_\alpha(\mathbf{r}')|^4}{\|\Phi_\alpha\|^4}\right]\Phi_\alpha(\mathbf{r}) + dW_\alpha(\mathbf{r}), \quad (1.10)$$

starting from the common value $\Phi_\alpha(\tau = 0)$ uniformly distributed on the unit sphere $\|\Phi_\alpha\| = 1$. The statistically independent noises $dW_\alpha(\mathbf{r})$ satisfy

$$\langle dW_\alpha(\mathbf{r})\, dW_\alpha(\mathbf{r}')\rangle = -\frac{g_0 d\tau}{2dV}\sum_{\mathbf{r}''}(Q_\Phi)_{\mathbf{r}\mathbf{r}''}(Q_\Phi)_{\mathbf{r}'\mathbf{r}''}\Phi_\alpha^2(\mathbf{r}''), \quad (1.11)$$

where we recall that the projector Q_Φ projects orthogonally to Φ [24].

A similar procedure can be used for real time evolution, in which case the Ito stochastic process is the same but for the replacement $-d\tau/2 \to dt/i\hbar$ [25, 35]. It is interesting to note that in contrast to the Positive-P representation [36], the Ito equations of the present exact method fulfill the hypothesis of a theorem ensuring that the stochastic trajectories cannot escape to infinity within a finite time [25].

Related stochastic schemes were developed in [37] starting from a Gutzwiller ansatz instead of the Fock state $|N : \Phi\rangle$. A different perspective on these methods is reviewed in P. Drummond's chapter (Chapter **??**). Interestingly, similar methods also apply to Fermi gases [38–40] (see also Chapter **??**).

An approximate semiclassical scheme to sample the thermal equilibrium state can be obtained by simply dropping the stochastic noise term in Eqs. (1.10) and replacing the bare coupling constant g_0 with the effective one g. As discussed in detail in [23], this is exact for the ideal gas and, for the interacting gas, it is one order more accurate in the high temperature expansion than the classical field.

1.3. Validity Issues

We summarize in Table 1.1 the validity conditions for the methods we present, where d is the dimension of space, $t_{\rm evol}$ and $t_{\rm therm}$ represent real evolution and thermalisation times, $\mathcal{N}$ is the number of modes and ξ is the healing length. As shown in [29], the Wigner method and the time-dependent Bogoliubov theory lead to the same one-body density operator up to order $O(N^{-1/2})$ excluded. The semiclassical method is for equilibrium only. The exact method has no restrictions but the computational effort grows exponentially with N and $t_{\rm evol}$.

Table 1.1. Summary of the validity conditions for all the methods.

Method	N	T	ξ	$t_{\rm evol}$
Wigner	$N \gg \frac{\mathcal{N}}{2}$	$T \ll T_c$	$\rho\xi^d \gg 1$	$t_{\rm evol} < t_{\rm therm}$
Classical field	$N \gg 1$	$k_B T \gg \lvert\mu\rvert$	$\rho\xi^d \gg 1$	–
Semiclassical	$N \gg 1$	$k_B T > \lvert\mu\rvert$	$\rho\xi^d \gg 1$	$t_{\rm evol} = 0$
Exact	–	–	–	–

1.3.1. *Relevance to other (non U(1)-symmetry preserving) theories*

A key advantage of our approaches for finite size systems is that they do not break the $U(1)$ symmetry. While the substitution of the condensate mode operator by a c-number was rigorously justified in the thermodynamic limit [41, 42], there is no spontaneous symmetry breaking in finite size systems. For these finite size systems the most natural and flexible approach is to work in the canonical ensemble where the total atom number is fixed. The initial quantum state of the system is then completely characterized by the density operator $\rho = Z^{-1}\exp(-\beta H)$ which is directly sampled. If necessary, fluctuations in the total atom number can be accounted for by further averaging. In practice, there are physical situations that are strongly affected by fluctuations in the total particle number, such as, in interacting Bose-Einstein condensates, the condensate phase spreading, the condensate number fluctuations, and the dynamical creation of Schrödinger cat states. For these situations, which may require an experimental control of the total atom number, a number-conserving theory has crucial advantages.

1.4. Applications

1.4.1. *Number Conserving Wigner Method*

Applications of the number-conserving Wigner method are shown in Fig. 1.1. Fig. 1.1(a), from [29], is an equilibrium result : it shows good agreement of the probability distribution of the number of condensate particles N_c in the canonical ensemble for a 1d harmonically trapped interacting Bose gas with Bogoliubov theory. Fig. 1.1(b), from [43], is a dynamical application of the Wigner method in the perturbative regime. The correlation pattern of density fluctuations $g^{(2)}(x,x') - 1 = \langle\hat\Psi^\dagger(x)\,\hat\Psi^\dagger(x')\,\hat\Psi(x')\,\hat\Psi(x)\rangle / \left(\rho(x)\,\rho(x')\right) - 1$ across a sonic horizon is shown in a flowing 1d condensate: in the $x < 0$ ($x > 0$) regions, the flow is respectively subsonic (supersonic). The three highlighted features are as follows: (i) is the anti-bunching due to repulsive interactions; (ii) stems from a dynamical Casimir emission of phonons at the horizon formation time; (iii) corre-

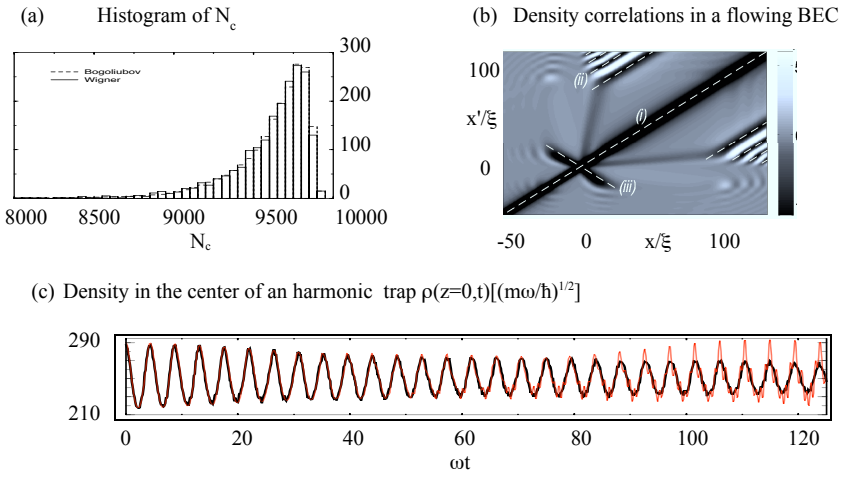

Fig. 1.1. (a) Probability of the number of condensate particles for a 1d trapped interacting Bose gas with $N = 10^4$, $k_BT = 30\hbar\omega$, $\mu_{\rm GP} = 14.1\hbar\omega$ (see text). Dashed line: Bogoliubov. Full line: Wigner. (Image from [29]). (b) Wigner method in the perturbative regime: Correlation pattern of density fluctuations $g^{(2)}(x, x') - 1$ across a sonic horizon in a flowing one-dimensional Bose-Einstein condensate. In the $x < 0$ ($x > 0$) regions, the flow is subsonic (supersonic). The greyscale from dark to bright is $[-5, 5]\times 10^{-3}$. Features (i), (ii) and (iii) are explained in the text. ξ is the healing length in the subsonic region. (Image from [43]). (c) Collapse of the oscillations of the mean density in the center of a 1d condensed cloud in a harmonic trap after an abrupt change of the trap frequency $\omega \to 0.8\omega$ ($k_BT = 30\hbar\omega$, $\mu_{\rm GP} = 3.1\hbar\omega$ and $N = 10^3$). Gray line: Bogoliubov. Black line: Wigner. (Image from [6]).

sponds to the continuous emission of correlated pairs of phonons by the horizon and can be interpreted as an acoustic analog of Hawking radiation [44, 45]. Finally Fig. 1.1(c), from [6], is a non-equilibrium application showing the superiority of Wigner to Bogoliubov in the nonperturbative regime. We show a collapse in the oscillations of the *mean* density in the center of a 1d harmonically trapped cloud after an abrupt reduction of the trap frequency. While Bogoliubov theory (gray line) correctly predicts the collapse at short times, it gives unphysically large oscillations at longer times due to an unlimited growth of the number of noncondensed particles, a side effect of the linearized treatment of the non-condensed field. This artifact of unlimited growth of $N - N_c$ may be eliminated by self-consistent number-conserving theories [46], which is particularly crucial in the case of a dynamic instability [47].

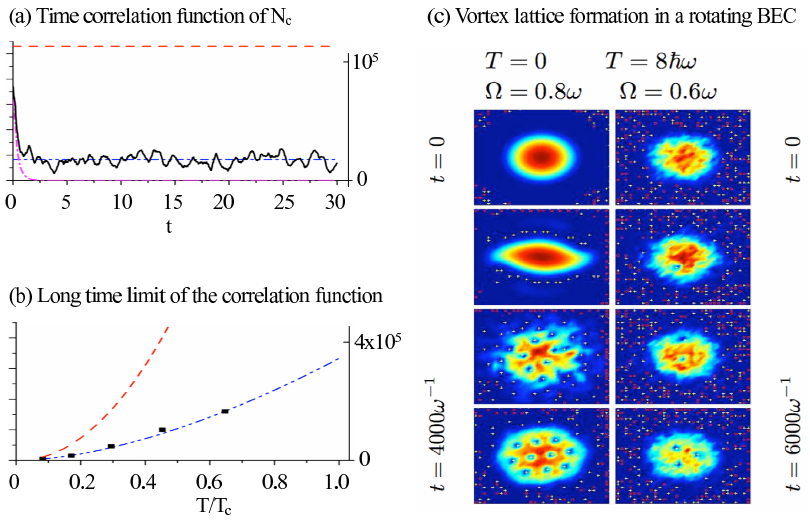

Fig. 1.2. (a) Correlation function of the condensate particle number $\langle N_c(t)N_c(0)\rangle - \langle N_c\rangle^2$ for a 3d homogeneous gas, or equivalently of the non-condensed particle number $N - N_c$ since the total number N is conserved. Time t is in units of $mV^{2/3}/\hbar$. ($N = 4\times10^5$, $gN/V = 700\hbar/mV^{2/3}$, $k_BT = 3077\hbar/mV^{2/3} = 0.1711T_c$, where T_c the critical temperature of the ideal gas). (Image from [1]). (b) Long time limit of the correlation function, as a function of T/T_c. Dashed lines: Bogoliubov. Dash-dotted line rapidly dropping to zero in (a): Gaussian model that includes the damping of the non-condensed field coherence fonction $\langle\Lambda^*(\mathbf{r},t)\Lambda(\mathbf{r}',0)\rangle$ due to Beliaev-Landau processes and that predicts a damping to zero of the correlation function of $N - N_c = dV\sum_{\mathbf{r}}\Lambda^*(\mathbf{r})\Lambda(\mathbf{r})$ using Wick's theorem. Dash-dot-dotted lines: Ergodic theory. Solid line in (a) and squares in (b): Classical field simulations with $N = 4\times10^5$, $gN/V = 700\hbar/mV^{2/3}$. (Image from [1]). We find quantitative agreement between the classical field simulations and the ergodic theory that predicts a *non-zero* long time limit of the correlation function for the system prepared in the canonical ensemble (see text). (c) Vortex lattice formation in a 3d Bose gas for a trap rotation frequency slowly ramped from 0 to Ω: Spatial density in the plane $z = 0$ at different times. Crosses (circles) indicate positions of vortices of positive (negative) charge. Left column ($T = 0$), top to bottom: Initial state; near instability; turbulent behaviour; end of simulation. Right column ($k_BT = 8\hbar\omega$), top to bottom: Initial state; entry of first vortex; entry of second vortex; end of simulation with a 3-vortex lattice. (Image from [14]).

1.4.2. *Classical Field Method*

Two applications of the classical field method in 3d are shown in Fig. 1.2 In Fig. 1.2(a), from [1], we show the temporal correlation function of the condensate atom number N_c in a homogeneous gas prepared at $T < T_c$ with a fixed total number of particles. The classical field results (black line in (a) and squares in (b)) are used as an exact model to test different analytic theories. These simulations show that, for a Bose condensed gas prepared at time zero in the canonical ensemble and totally isolated in its further evolution, the temporal correlation function of

N_c between times 0 and t does not tend to zero in the long t limit, contrarily to the intuition and to the *a priori* reasonable assumption that the non-condensed fields $\Lambda(\mathbf{r}, 0)$ and $\Lambda(\mathbf{r}', t)$, that experience decoherence due to the Beliaev-Landau mechanism, obey Gaussian statistics. The explanation given in [1] involves three key ingredients, energy fluctuations in the initially prepared state, energy conservation in the later time evolution (hence the failure of the Gaussian model in Fig. 1.2(a)), and ergodicity due to interactions among the Bogoliubovs modes at the origin of the Beliaev-Landau processes (hence the failure of the usual Bogoliubov theory in Fig. 1.2(a) and (b), that neglects such interactions). This counterintuitive result of an infinite correlation time for the condensate particle number N_c indicates that the non-condensed modes cannot always be correctly treated as a simple heat bath for the condensate [48–50]. The classical field method was also used to test a kinetic theory calculation of the microcanonical condensate phase diffusion coefficient [2]. In Fig. 1.2(c), from [14], the classical field method is applied to the problem of vortex lattice formation in a rotating condensed gas initially at zero (left column) and finite temperature (right column). The full nonlinearity contained in the classical field allows the transfer of energy from collective to microscopic degrees of freedom, which is effective purely Hamiltonian dissipation, and the consequent crystallization of the vortex lattice. This validates the scenario of vortex lattice formation by dynamic instability of hydrodynamic modes proposed in [51] and experimentally tested in [52]. Similar classical field results were obtained in 2d, with a quantitative study of the induced turbulence [53]. More recently we have used a mixed classical field and Wigner method to determine the limit to spin squeezing in a finite temperature interacting Bose-Einstein condensate [11].

1.4.3. *Exact and Semiclassical Methods*

We show two equilibrium applications of the exact and the semiclassical methods in Fig. 1.3. Fig. 1.3(a), from [54], shows the exact probability distribution $P(N_c)$ of the number of condensate atoms for decreasing temperatures for a 1d system of $N = 125$ atoms in a harmonic trap:

$$P(N_c) = \frac{N!}{N_c!(N-N_c)!}\langle (c_2^* c_1)^{N_c} (\langle \Phi_2^\perp | \Phi_1^\perp \rangle)^{N-N_c} \rangle_{\text{stoch}} \tag{1.12}$$

where the stochastic fields of the exact method are split in components parallel and orthogonal to the exact condensate mode, $\Phi_\alpha(\mathbf{r}) = c_\alpha \phi_{\text{exact}}(\mathbf{r}) + \Phi_\alpha^\perp(\mathbf{r})$. ϕ_{exact}, normalized to unity, is obtained as the most populated eigenstate of the exact one-body density operator $\rho_1 = \langle |\Phi_1\rangle\langle\Phi_2| (\langle \Phi_2 | \Phi_1 \rangle)^{N-1} \rangle_{\text{stoch}}$. In Fig. 1.3(b), from [23], the semiclassical method is applied to Berezinskii-Kosterlitz-Thouless physics in

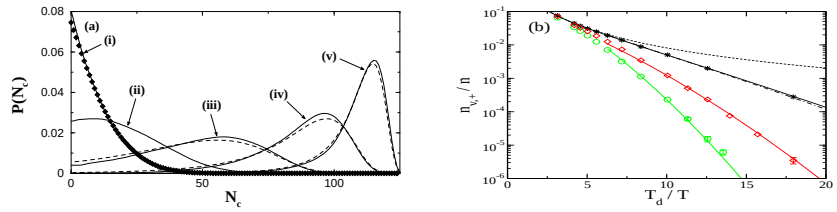

Fig. 1.3. (a) Exact probability distribution $P(N_c)$ of the number of condensate atoms in a 1d Bose gas with $N = 125$ for temperatures $k_BT/\hbar\omega = 50$ (i), 33 (ii), 20 (iii), 10 (iv), 5 (v). The 1d coupling constant is $g_0 = 0.08\hbar(\hbar\omega/m)^{1/2}$. Dashed lines in curves (iii,iv,v): Bogoliubov. Diamonds in curve (i): ideal gas. (Image from [54]). (b) Temperature dependence of the mean density of positive charge vortices in a homogeneous 2d Bose gas, denoted by $n_{v,+}$ with $N = 1000$. The degeneracy temperature is $T_d = 2\pi\hbar^2\rho/m$. (The surface density ρ is called n in the figure). Symbols from top to bottom: semiclassical simulations for coupling constants $g = 0$, $g = 0.1\hbar^2/m$, $g = 0.3\hbar^2/m$. Solid lines: exact canonical result for $g = 0$; analytical prediction of an activation law $n_{v,+}/n = Ce^{-\Delta(T)/k_BT}$ for $g \neq 0$. $\Delta(T)$ is the minimal energy to create a node in the field Φ for a temperature dependent semiclassical energy functional, hence a (in 2d logarithmic) dependence of Δ on T. Dot-dashed line (barely distinguishable from the $g = 0$ solid line): Bogoliubov for $g = 0$. Dashed line: grand canonical result for $g = 0$, which totally differs from the $g = 0$ canonical result, due to large unphysical fluctuations of the condensate particle number in the grand canonical ensemble [55, 56]. (Image from [23]).

a 2d homogeneous Bose gas. The mean density of positive charge vortices is calculated as a function of temperature for various interaction strengths and compared with analytical predictions (see the caption of the figure).

Keywords

bosons; canonical ensemble; classical field; exact method; number conserving; semiclassical field method; truncated Wigner.

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