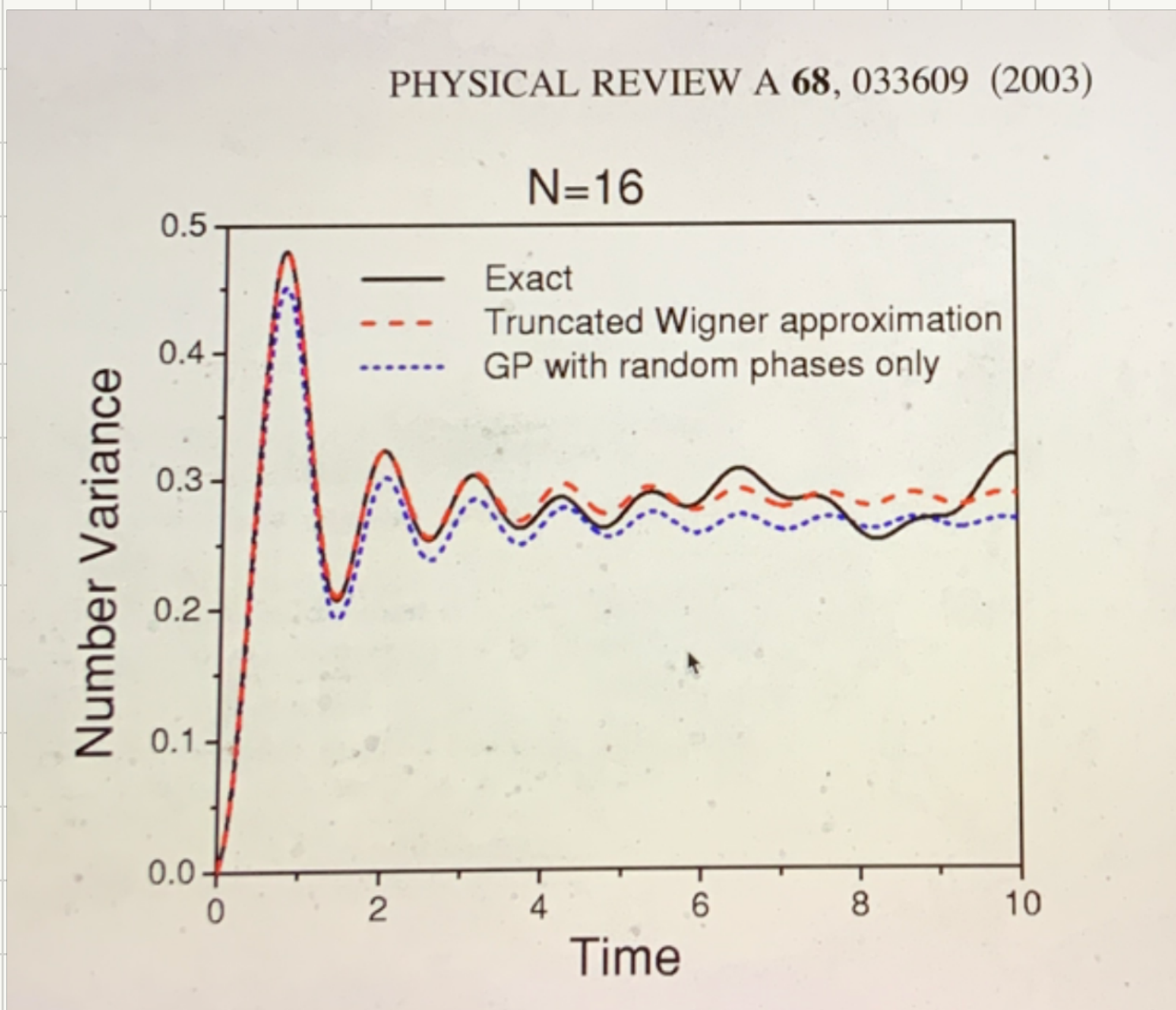


W_0 is not positive and thus one has to numerically solve eqs. (263) and subsequently numerically integrate over W_0 .



GP corresponds to the mean-field result. One recognizes a rather good agreement for a number of tunneling times.

VI.3 Truncated Wigner approximation to trapped, multi-mode Bose gases

We now want to discuss the application of the TWA to multi-mode ultra-cold Bose gases at finite T .

We follow here Sinatra, Lobo, Cashin J. Phys. B 35
(2002) 3599

(A) Basic notation and assumptions

Since we have consider a continuous Bose field $\hat{\psi}(\vec{r})$ symmetric ordering poses a problem. E.g.

$$\begin{aligned} \hat{\psi}^\dagger(x) \hat{\psi}(x') &= \left(\hat{\psi}^\dagger(x) \hat{\psi}(x') \right)_{\text{sym}} \\ (268) \quad &- \frac{1}{2} \underbrace{\left[\hat{\psi}(x'), \hat{\psi}^\dagger(x) \right]}_{= \delta^{(3)}(x-x')} \quad \Downarrow \end{aligned}$$

i.e. for $x' = x$ we have $\delta^{(3)}(0) = \infty$

Physically this stems from the vacuum fluctuations in every mode

$\Rightarrow$ discretization and truncation of modes

Consider discrete spatial grid in box of length L_μ $\mu = x, y, z$

of grid points N_μ and periodic BC

$$(269) \quad V = L_x L_y L_z \quad \mathcal{N} = N_x N_y N_z$$

decomposition into plane waves

$$(270) \quad \hat{\psi}(\vec{r}_j) = \sum_{\mathbf{k}} \frac{1}{\sqrt{V}} \hat{a}_{\mathbf{k}} e^{i\vec{k}\cdot\vec{r}_j} \quad k_{\mu} = \frac{2\pi}{L_{\mu}} j_{\mu}$$

$$j_{\mu} = -\frac{n_{\mu}}{2}, \dots, \frac{n_{\mu}}{2} \quad (n_{\mu} : \text{even})$$

remark: for trapped gases $\Rightarrow$ decomposition into trap modes

$$(271) \quad \hat{a}_{\mathbf{k}} = dV \sum_{\vec{r}} \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}} \hat{\psi}(\vec{r}) \quad dV = \frac{V}{\mathcal{N}}$$

In this approximation

$$(272) \quad [\hat{\psi}(\vec{r}_i), \hat{\psi}^{\dagger}(\vec{r}_j)] = \frac{1}{dV} \delta_{ij}$$

With this we have

$$(273) \quad \langle \hat{\psi}^{\dagger}(x) \hat{\psi}(x) \rangle = \langle \psi^*(x) \psi(x) \rangle_w - \frac{1}{2} \frac{1}{dV}$$

and similarly for higher-order correlations.

The multi-mode Wigner function can now be obtained from the characteristic function

$$(274) \quad \chi_w(\gamma(\vec{r})) = \text{Tr} \left[\rho \exp \left\{ dV \sum_{\vec{r}} \left(\gamma(\vec{r}) \hat{\psi}^{\dagger}(\vec{r}) - \gamma^*(\vec{r}) \hat{\psi}(\vec{r}) \right) \right\} \right]$$

where $\sum_{\vec{r}}$ is over the discrete space points

$$(275) \quad W(\psi) = dV \prod_r \left[\int \frac{d^2 \psi(r)}{\pi^2} \right] \chi(\psi) e^{dV \sum_r (\psi^* \psi - \psi \psi^*)}$$

With the normalization

$$(276) \quad dV \prod_r \int d^2 \psi(r) W(\psi) = 1$$

expectation values of operators

$$(277) \quad \langle O_1 \cdots O_n \rangle_w \equiv \frac{1}{n!} \sum_{\text{perm.}} \text{Tr} \{ S \hat{O}_{P(1)} \cdots \hat{O}_{P(n)} \}$$

Wigner average operator average

where the Wigner average is

$$(278) \quad \langle O \rangle_w = dV \prod_r \int d^2 \psi(r) W(\psi) O(\psi)$$

Symmetric ordering and Bopp-operators

The evaluation of operator averages in terms of Wigner averages $\langle \cdots \rangle_w$ can be cumbersome. For this the following relation is useful

$$(279) \quad \begin{aligned} \hat{\psi}(\vec{r}) &\equiv \psi(\vec{r}) + \frac{1}{2} \frac{\delta}{\delta \psi^*(\vec{r})} \\ \hat{\psi}^\dagger(\vec{r}) &\equiv \psi^*(\vec{r}) - \frac{1}{2} \frac{\delta}{\delta \psi(\vec{r})} \end{aligned}$$

Bopp
operators

$$(280) \quad \boxed{\langle f(\hat{\psi}^\dagger, \hat{\psi}) \rangle = \left\langle f\left(\psi^* - \frac{1}{2} \frac{\delta}{\delta \psi}, \psi + \frac{1}{2} \frac{\delta}{\delta \psi^*}\right) \mathbb{1} \right\rangle_w}$$

E.g.

$$(281) \quad \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}') \rangle = \left\langle \left(\psi^*(\vec{r}) - \frac{1}{2} \frac{\delta}{\delta \psi(\vec{r})} \right) \left(\psi(\vec{r}') + \frac{1}{2} \frac{\delta}{\delta \psi^*(\vec{r}')} \right) \right\rangle_w$$

$\delta^{(3)}(\vec{r} - \vec{r}')$

$$= \langle \psi^*(\vec{r}) \psi(\vec{r}') \rangle_w - \frac{1}{2} \delta^{(3)}(\vec{r} - \vec{r}')$$

or

$$(282) \quad \langle \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) \hat{\psi}(y') \hat{\psi}(x') \rangle =$$

$$= \left\langle \left(\psi^*(x) - \frac{1}{2} \frac{\delta}{\delta \psi(x)} \right) \left(\psi^*(y) - \frac{1}{2} \frac{\delta}{\delta \psi(y)} \right) \left(\psi(y') + \frac{1}{2} \frac{\delta}{\delta \psi^*(y')} \right) \left(\psi(x') + \frac{1}{2} \frac{\delta}{\delta \psi^*(x')} \right) \right\rangle_w$$

$\delta(x-y')$

$\delta(y-y')$

$\delta(x-x')$

$$= \langle \psi^*(x) \psi^*(y) \psi(y') \psi(x') \rangle_w - \frac{1}{2} \delta(x-x') \langle \psi^*(y) \psi(y') \rangle_w$$

$$- \frac{1}{2} \delta(x-y') \langle \psi^*(y) \psi(x') \rangle - \frac{1}{2} \delta(y-x') \langle \psi^*(x) \psi(y') \rangle_w$$

$$- \frac{1}{2} \delta(y-y') \langle \psi^*(x) \psi(x') \rangle + \frac{1}{4} \delta(x-x') \delta(y-y')$$

$$+ \frac{1}{4} \delta(x-y') \delta(y-x')$$

Mode truncation replaces the δ -functions by Kronecker δ

$$(283) \quad \delta(x_i - x_j) \rightarrow \frac{1}{dV} \delta_{ij}$$

For the special case of $x = x'$ and $y = y'$ and using the mode truncation yields for the second order correlation

$$(284) \quad \langle \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}(x) \rangle = \\ = \langle \hat{\psi}^*(x) \hat{\psi}^*(x) \hat{\psi}(x) \hat{\psi}(x) \rangle_w - \frac{2}{dV} \langle \hat{\psi}^*(x) \hat{\psi}(x) \rangle_w \\ + \frac{1}{2} \frac{1}{dV} \quad \text{etc.}$$

Weakly interacting BEC

Hamiltonian of weakly interacting Bose gas in S-wave scattering approximation, eq. (46):

$$(285) \quad \hat{H} = \int d^3\vec{r} \hat{\psi}^\dagger(\vec{r}) \left[-\frac{\hbar^2}{2m} \Delta + V(\vec{r}) \right] \hat{\psi}(\vec{r}) \\ + \frac{g}{2} \int d^3\vec{r} \hat{\psi}^\dagger(\vec{r}) \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \hat{\psi}(\vec{r})$$

In chapter II we have seen that approximating the ground state by a (multimode) coherent state leads to the Gross-Pitaevski equation for the coh. amplitude

$$(286) \left(-\frac{\hbar^2}{2m} \Delta + V(\vec{r}) + g |\psi(\vec{r})|^2 \right) \psi(\vec{r}) = \mu \psi(\vec{r})$$

Where μ is the chemical potential. Here we see that we can introduce a characteristic length scale associated with the interactions

$$\frac{\hbar^2}{2m \xi^2} = g |\psi(\vec{r})|^2 \approx g n$$

$$(287) \quad \boxed{\xi = \frac{\hbar}{\sqrt{2m g n}}} \quad \text{healing length}$$

with n being the characteristic density of the BEC.

The chosen spatial grid size dx_v in (271) must be small compared to the physical length scales

$$(288) \quad dx_v \ll \xi \quad dx_v \ll \lambda_{th}$$

where $\lambda_{th} = \sqrt{\frac{2\pi \hbar^2}{m k_B T}}$ is the thermal de Broglie wavelength.

Using the mappings between operator products and the Wigner function yields the following eq. of motion of W

$$\frac{\partial}{\partial t} \rho = -\frac{i}{\hbar} [H, \rho] \Rightarrow$$

$$(289) \quad i\hbar \frac{\partial}{\partial t} W = \sum_r \left\{ \frac{\partial}{\partial \psi(r)} (-f_\psi W) + \frac{g}{4(dV)^2} \frac{\partial^3}{\partial^2 \psi(\bar{r}) \partial \psi^*(\bar{r})} \psi(\bar{r}) W + c.c. \right\}$$

Where f_ψ defines the drift term

$$(290) \quad f_\psi = \left(-\frac{\hbar^2}{2m} \Delta + V(\bar{r}) + g |\psi(\bar{r})|^2 - \frac{g}{dV} \right) \psi$$

The truncated Wigner approximation consist in neglecting the third-order derivative in eq. (289)

$$(291) \quad i\hbar \frac{\partial}{\partial t} W = - \sum_r \frac{\partial}{\partial \psi(r)} f_\psi W$$

This is then equivalent to a stochastic field ψ obeying the time-dependent GPE

$$(292) \quad i\hbar \frac{\partial}{\partial t} \psi = \left(-\frac{\hbar^2}{2m} \Delta + V(\vec{r}) + g |\psi(\vec{r})|^2 - \frac{g}{dV} \right) \psi$$

The term $-\frac{g}{dV}$ resulting from the symmetric ordering has no dynamical consequence and can be dropped. Different from the variational approach in Sec. II, $\psi(\vec{r})$ is the Wigner field and we have to average its initial conditions over the initial Wigner distribution. As we will see this

includes lowest-order quantum fluctuations

(B) Bose condensed gas in thermal equilibrium
- particle number conserving Bogoliubov
theory and Wigner representation

For a Bose gas below the condensation temperature we can assume a macroscopic occupation of a single condensate mode $\phi(\vec{r})$ obeying the stationary GPE (105)

$$(293) \quad \left(-\frac{\hbar^2}{2m} \Delta + V(\vec{r}) + g N |\phi|^2 \right) \phi = \mu \phi$$

where
(284)

$$\int d^3r |\phi(r)|^2 = 1$$

i.e. we separated the total number of particles N

Thus we split the full quantum field into a condensed and a non-condensed part

(295)

$$\hat{\psi}(\vec{r}) = \phi(\vec{r}) \hat{a}_\phi + \hat{\psi}_\perp(\vec{r})$$

Remark: the commonly used Bogoliubov approximation treats $\hat{a}_\phi$ as a c-number

$$\hat{a}_\phi = \sqrt{N_0}$$

which breaks the $U(1)$ symmetry of the problem

Here we keep the operator character, however!

(296)

$$\hat{a}_\phi = e^{i\theta} (\hat{N}_0)^{1/2} = \hat{A}_\theta (\hat{N}_0)^{1/2}$$

where $\hat{N}_0$ is the number operator in the condensate mode and

(297)

$$\hat{A}_\theta \equiv e^{i\theta}$$

$$\hat{A}_\theta \hat{A}_\theta^\dagger = \hat{A}_\theta^\dagger \hat{A}_\theta = \mathbb{1}$$

is the condensate phase operator. For a fixed total number N of particles we have

(298)

$$\hat{N}_0 = N - \int d^3r \hat{\psi}_\perp^\dagger \hat{\psi}_\perp$$

In the following it is convenient to use the modified field operator for the non-condensed atoms

(299)

$$\hat{\psi}_\perp(\vec{r}) \rightarrow \hat{\psi}(\vec{r}) \equiv \hat{A}_0^\dagger \hat{\psi}_\perp(\vec{r})$$

Substituting the expansion (295) into the Many-body Hamiltonian (285) reproduces the GP term plus a term in second and higher orders in $\hat{\psi}$. Terms linear in $\hat{\psi}$ vanish!

Neglecting terms $\mathcal{O}(\hat{\psi}^3)$ results in a quadratic Hamiltonian in $\hat{\psi}$

Bogoliubov approximation

(300)

$$H_B(\hat{\psi}) = \frac{1}{2} \int_V d^3r (\hat{\psi}^\dagger, -\hat{\psi}) \cdot \underline{h} \begin{pmatrix} \hat{\psi} \\ \hat{\psi}^\dagger \end{pmatrix}$$

where

(301)

$$\underline{h} = \begin{pmatrix} H_{GP} + Q g N |\phi|^2 Q & Q g N \phi^2 Q^* \\ -Q^* g N \phi^{*2} Q & -H_{GP} - Q^* g N |\phi|^2 Q^* \end{pmatrix}$$

→ and Q projects to functions orthogonal to $\phi(x)$

The thermal state of the system in Bogoliubov approximation then simply reads

$$(302) \quad \mathcal{S}_T = \frac{1}{Z} \exp \left\{ - \frac{1}{k_B T} H_B(\hat{\mathcal{L}}) \right\}$$

The usual way to proceed would be to diagonalize $H_B(\hat{\mathcal{L}})$. To this end one has to solve the eigenvalue equation of L

$$(303) \quad \boxed{L \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \epsilon_k \begin{pmatrix} u_k \\ v_k \end{pmatrix}}$$

Bogoliubov
-de Gennes
equations
(BdG)

requiring orthogonality

$$(304) \quad \int_V d^3r \, u_k^*(\vec{r}) u_{k'}(\vec{r}) - v_k^*(\vec{r}) v_{k'}(\vec{r}) = \delta_{kk'}$$

Then the decomposition of the field $\hat{\mathcal{L}}(\vec{r})$

$$(305) \quad \boxed{\begin{pmatrix} \hat{\mathcal{L}}(\vec{r}) \\ \hat{\mathcal{L}}^\dagger(\vec{r}) \end{pmatrix} = \sum_k \hat{b}_k \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} + \hat{b}_k^\dagger \begin{pmatrix} v_k^*(\vec{r}) \\ u_k^*(\vec{r}) \end{pmatrix}}$$

yields the diagonal form

$$(306) \quad \boxed{H_B = E_0 + \sum_{\vec{k}} \epsilon_k \hat{b}_k^\dagger \hat{b}_k}$$

The new quasi-particles described by creation and annihilation operators $b_k^\dagger, b_k$ are called

Bogoliubov phonons

► In the absence of a trapping potential $V(\vec{r})$ and for periodic boundary conditions the Bogoliubov-de Gennes equations can be solved by plane waves and gives

$$(307) \quad \begin{aligned} u_k(\vec{r}) &= \frac{1}{\sqrt{V}} e^{i\vec{k}\vec{r}} \cosh \theta_k \\ v_k(\vec{r}) &= \frac{1}{\sqrt{V}} e^{-i\vec{k}\vec{r}} \sinh \theta_k \end{aligned}$$

where

$$(308) \quad \left. \begin{array}{l} \cosh \theta_k \\ \sinh \theta_k \end{array} \right\} = \sqrt{\frac{\frac{k^2}{2m} + gn \pm \omega_k}{2\omega_k}}$$

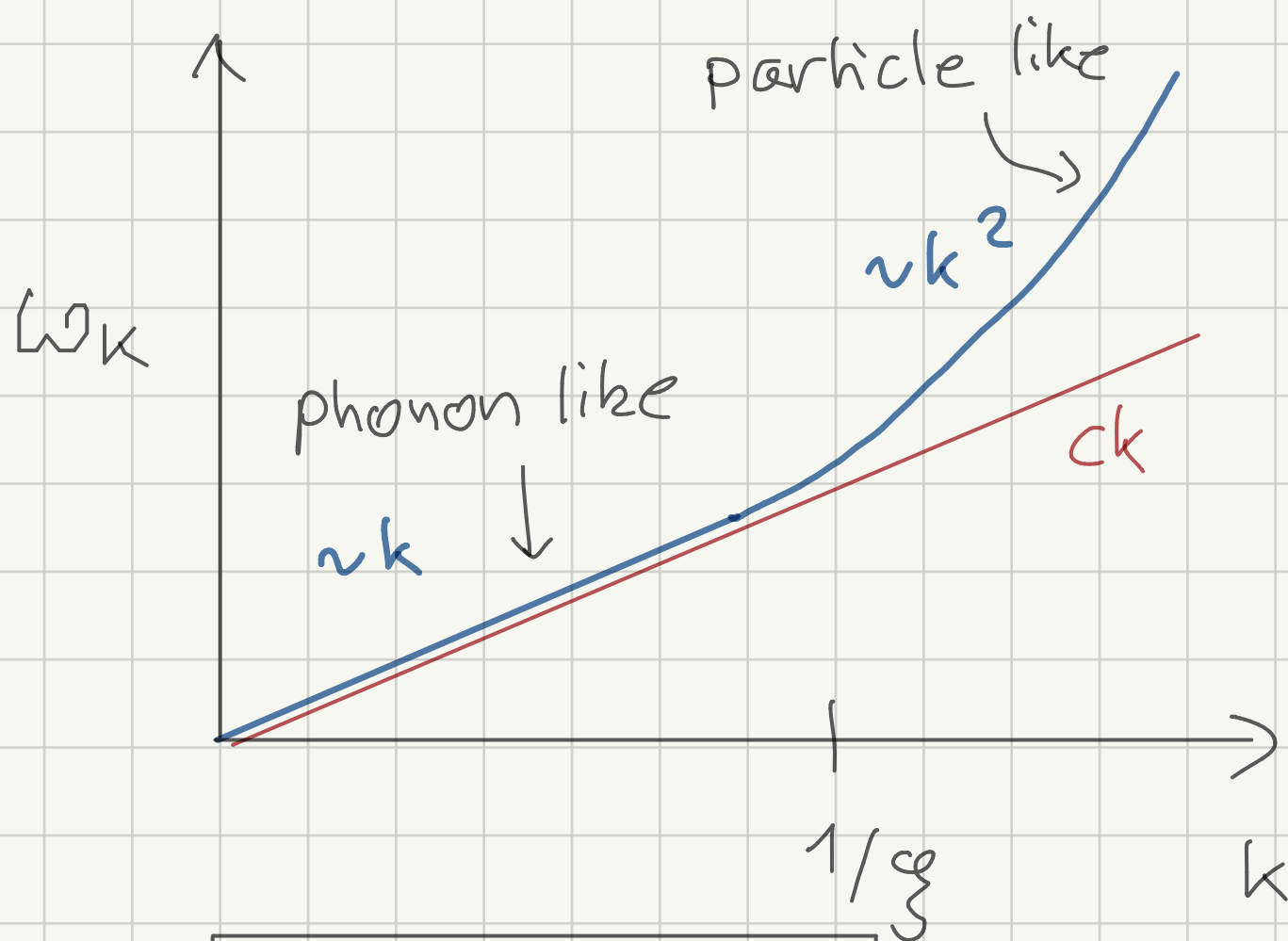
and

$$(309) \quad \omega_k = \frac{\epsilon_k}{\hbar} = \left[\left(\frac{k^2}{2m} + gn \right)^2 - (gn)^2 \right]^{1/2}$$

(309)

$$\omega_k = ck \sqrt{1 + k^2 \xi^2 / 2}$$

Bogoliubov spectrum



(310)
$$c = \sqrt{\frac{n g}{m}}$$
 speed of sound

► In the presence of a trapping potential $V(\vec{r})$ the solution of the BdG equations is numerically involved!

We will now show that the Wigner distribution of the thermal state $\mathcal{S}_{Th}$ can be obtained without solving the BdG equations!

Assume for a moment that we have solved the BdG equations, then the Wigner function of the complex mode amplitudes

$$W(\{\beta_k\}, \{\beta_k^*\})$$

is the $\mathcal{F}$ -trafo of the characteristic function,

$$(311) \quad \chi_w(\alpha_k, \alpha_k^*) = \text{Tr} \left\{ \mathcal{G}_T \prod_k \exp(\alpha_k \hat{b}_k - \alpha_k^* \hat{b}_k^*) \right\}$$

i.e.
(312)

$$W(\beta_k, \beta_k^*) = \left(\prod_k \int \frac{d\alpha_k}{\pi} \right) \chi_w(\alpha_k, \alpha_k^*) \exp(\alpha_k^* \beta_k - \alpha_k \beta_k^*)$$

The diagonalized Hamiltonian H_B , eq. (306), is a sum of uncoupled harmonic oscillators.

Thus the density operator $\mathcal{G}_T$ corresponds to uncoupled harmonic oscillators at thermal equilibrium. Thus (compare Sec. III)

$$(313) \quad W(\beta_k, \beta_k^*) = \prod_k 2 \tanh\left(\frac{\beta \varepsilon_k}{2}\right) \exp\left(-2 |\beta_k|^2 \tanh\left(\frac{\beta \varepsilon_k}{2}\right)\right)$$

Wigner function of non-condensed atoms

► Since we want to avoid the diagonalization by solving the BdG equations we now express (313) in terms of fields λ, λ^* corresponding to the field operators $\hat{\lambda}, \hat{\lambda}^*$

$$(314) \quad \begin{pmatrix} \lambda(\vec{r}) \\ \lambda^*(\vec{r}) \end{pmatrix} = \sum_k \beta_k \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} + \beta_k^* \begin{pmatrix} v_k^*(\vec{r}) \\ u_k^*(\vec{r}) \end{pmatrix}$$

Using the orthonormality of the $u_k(\vec{r})$ and $v_k(\vec{r})$ one finds

$$W(\lambda, \lambda^*) = N \exp \left\{ - \int d^3r (\lambda^*(r), \lambda(r)) \cdot \tilde{M} \begin{pmatrix} \lambda(r) \\ \lambda^*(r) \end{pmatrix} \right\}$$

(315)

$$= N \exp \left\{ - \int dV (\underline{\lambda}^*, \underline{\lambda}) \cdot M \begin{pmatrix} \underline{\lambda} \\ \underline{\lambda}^* \end{pmatrix} \right\}$$

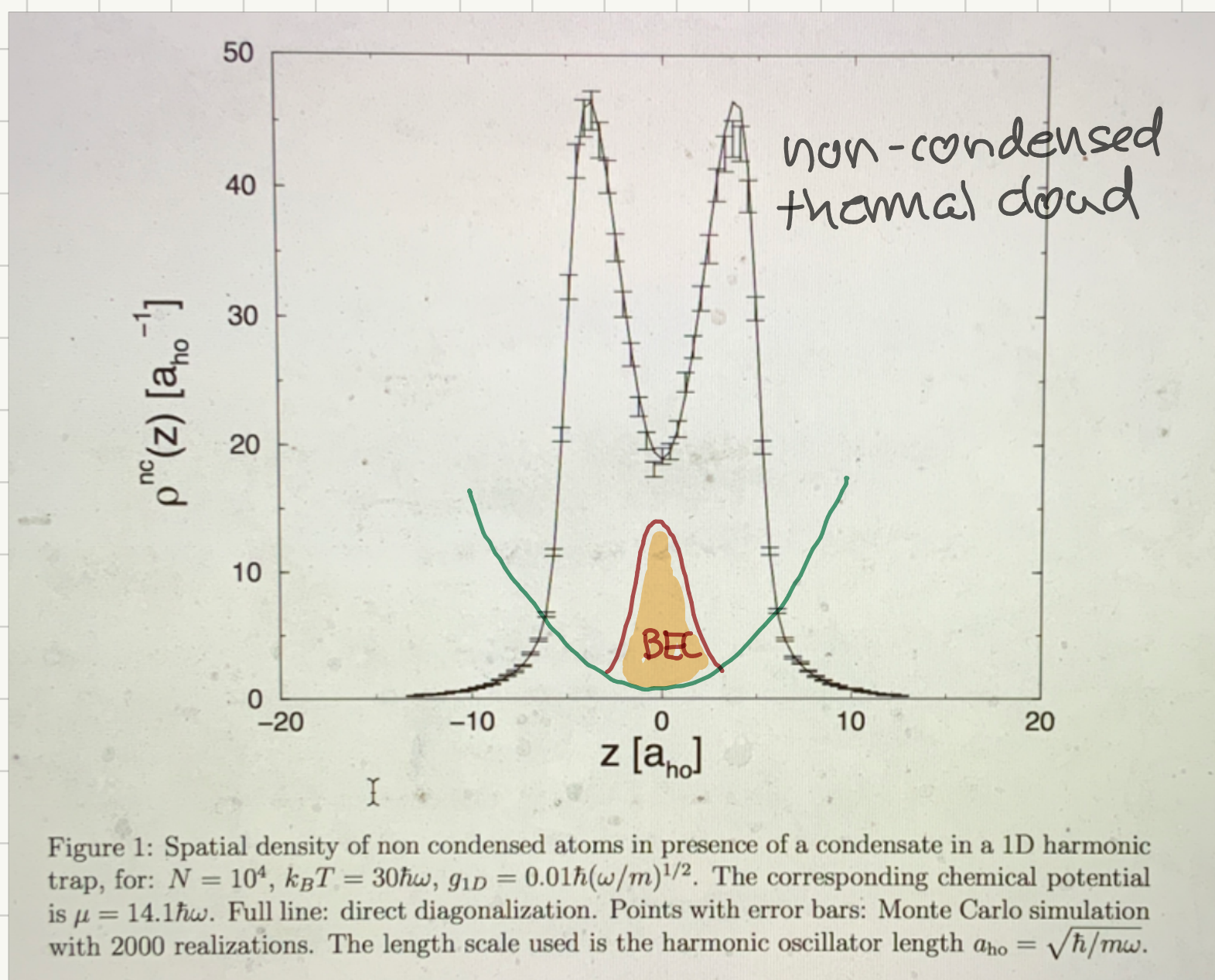
Wigner function of non-condensed atoms

where

$$(316) \quad M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tanh \left(\frac{\beta \hbar}{2} \right)$$

and h is the $2N \times 2N$ matrix of the discretized BdG Hamiltonian (301).

example: 1D condensate in harmonic trap



A. Sinatra

Y. Castin

J. Mod. Optics 47

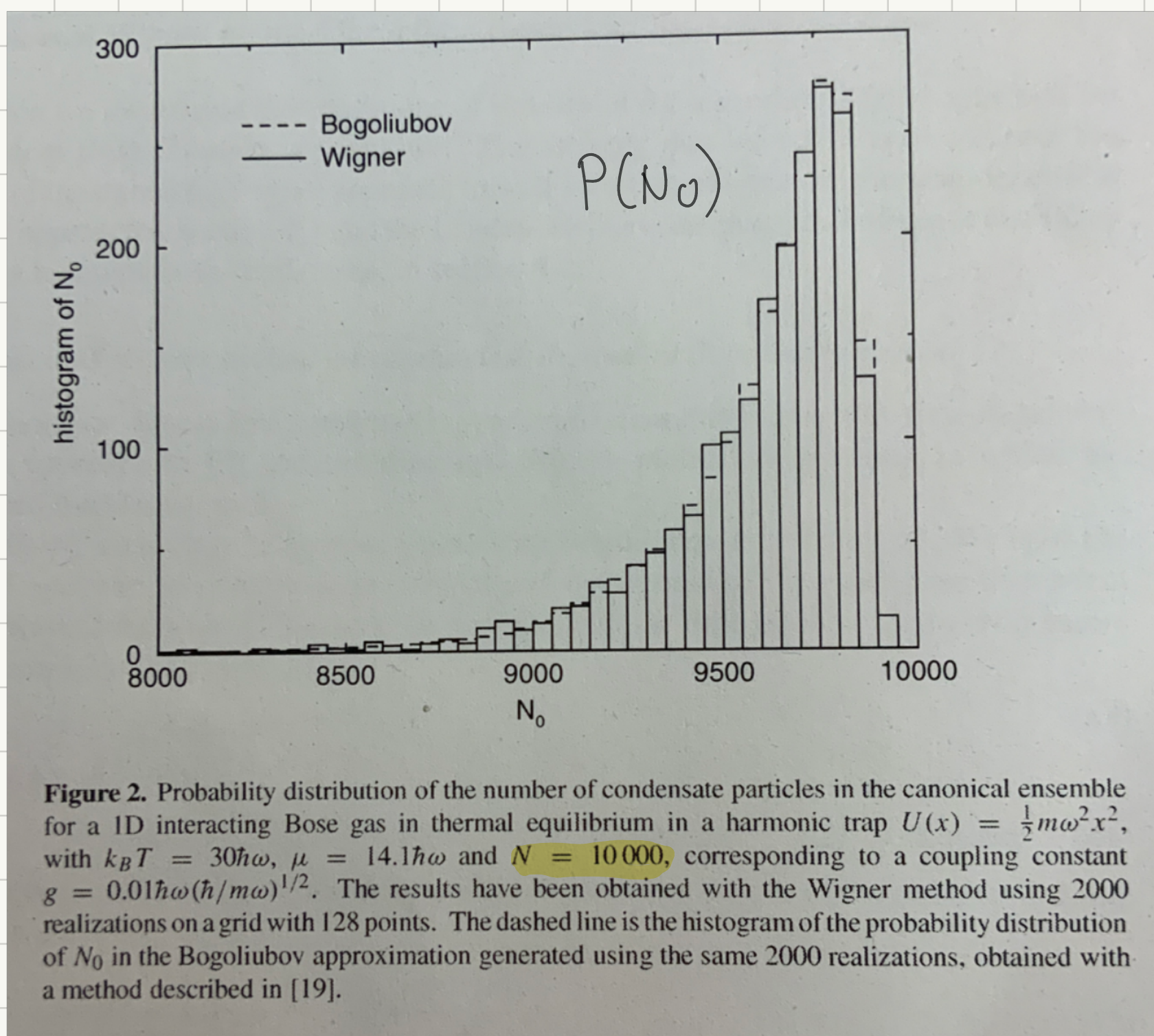
2629 (2000)

condensate field

The condensate is described by the wavefunction $\phi(\vec{r})$ and the particle number

$$(317) \quad \hat{N}_0 = N - \int d^3r \hat{\psi}_\perp^\dagger \hat{\psi}_\perp = N - \int d^3r \hat{\Lambda}^\dagger \hat{\Lambda}$$

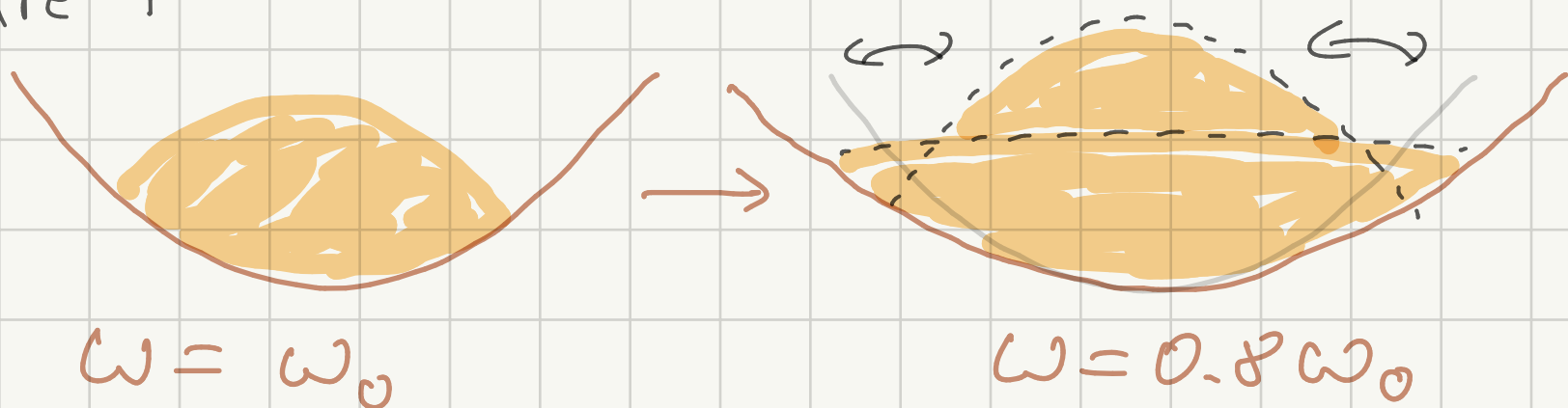
The probability distribution of the particle number in the condensate can be obtained from the distribution of particle number in the non-condensed field



Sinatra, Lobo, Cashin J. Phys. B 35, 3599 (2002)

(C) Truncated Wigner method for a time-dependent Bose condensed gas

Consider a one-dimensional trapped BEC at finite T



breathing oscillations

• Gross Pitavuski equation $\rightarrow$ undamped oscillations

• Bogoliubov $\hat{\psi}(x,t) = \sqrt{N_0} \phi(x,t) + \hat{\psi}_\perp(x,t)$
 $\Rightarrow$ damped oscillations

• TWA

larger damping at longer times

backaction to condensate

Landau damping

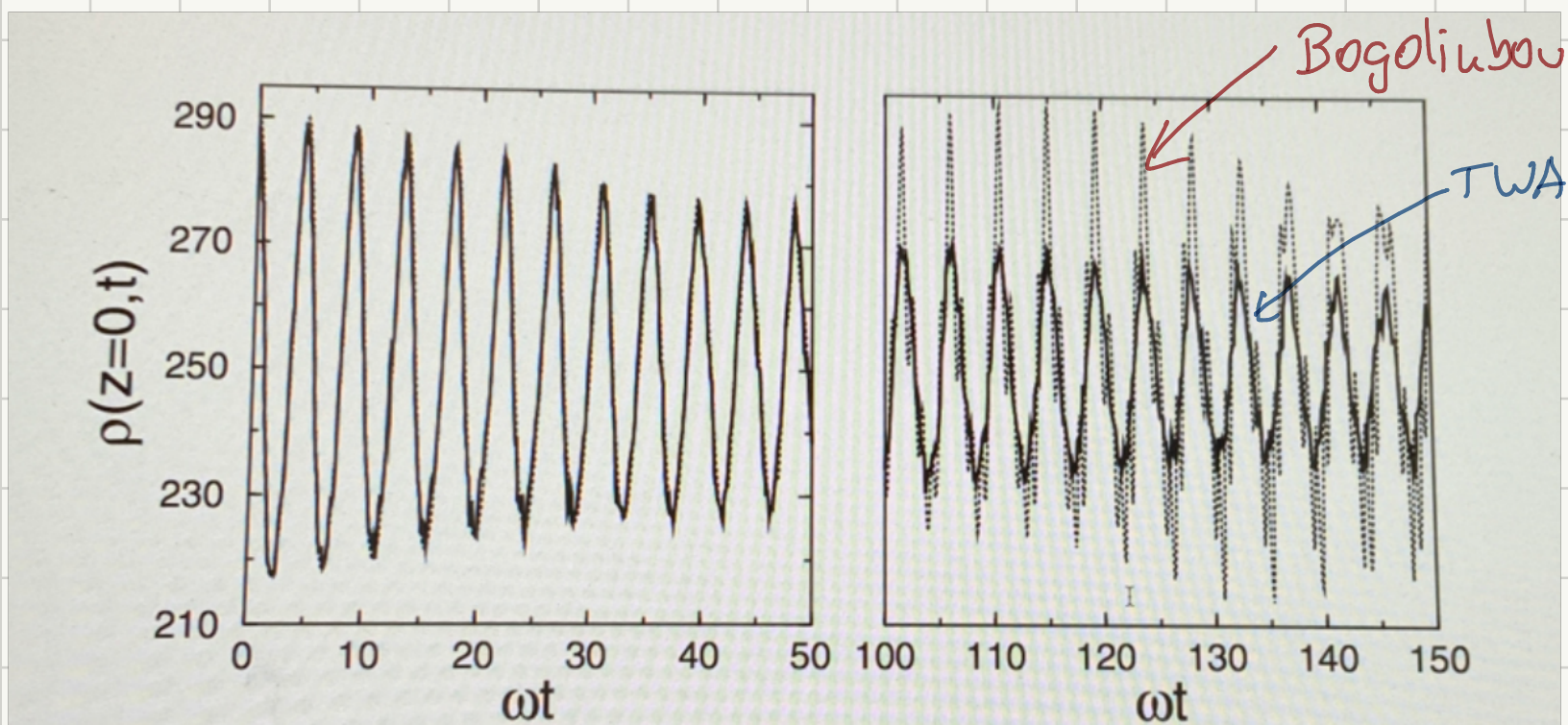


FIG. 1. Damped oscillations of the mean density in the center of a 1D condensed cloud in a harmonic trap after an abrupt change of the trap frequency $\omega \rightarrow 0.8\omega$. $k_B T = 30\hbar\omega$, $\mu = 3.1\hbar\omega$, and $N = 10^3$. Solid line: Wigner simulation. Dotted curve: Bogoliubov theory. ρ is in units of $(m\omega/\hbar)^{1/2}$.