Classical quasiparticle dynamics and chaos in trapped Bose condensates

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Abstract

In the short wavelength limit the Bogoliubov quasiparticles of trapped Bose-Einstein condensates can be described as classical particles and antiparticles with dynamics in a mixed phase-space. For anisotropic parabolic traps we determine the location of the resonances and study the influence of the sharpness of the condensate surface on the appearance of chaos as the energy of the quasiparticles is lowered from values much larger than to values comparable with the chemical potential.

I. INTRODUCTION

The achievement of Bose-Einstein condensation of clouds of magnetically trapped alkali atoms \[①\] by evaporation cooling to temperatures in the 100 nano-Kelvin regime has revived the interest in the physics of weakly interacting Bose-condensed gases. As is well-known the bulk properties of such gases are rather well described by ideal gases of quasiparticles, first derived microscopically by Bogoliubov \[②\], which are collisionless phonons at long wavelength and approach free particles at short wavelength. In the case of trapped

*dedicated to Boris Chirikov on the occasion of his 70th birthday
condensates of repelling atoms, to which we confine our discussion here, the quasiparticle
description retains its usefulness. However, trapped condensates are spatially inhomoge-
neous. They form around the minima of the trapping potential and can form rather sharp
surfaces. The thickness of the surface layer, given by the healing length \[ \xi \], can become
very small compared to the radius of the condensate. Quasiparticles may therefore leave the
condensate and reenter it after being reflected back by the trapping potential. Therefore
their dynamics are more complex than in a homogeneous system. In Bogoliubov’s approach
single quasiparticles are described by wavefunctions, which are solutions of a set of linear
wave equations. This is in complete analogy to the description of single particles in quan-
tum mechanics by Schrödinger’s equation. We know that it is extremely fruitful to examine
the classical limit of the Schrödinger equation, which gives all of classical physics. In the
same spirit we can examine the classical limit of the wave equations for the quasiparticles.
In spatially homogeneous condensates this gives a simple theory of free quasiparticles with
conserved momentum which are distinguished from free particles merely by their unusual
relation between energy and momentum, and hence also between velocity and momentum.

In the case of trapped inhomogeneous condensates recent work has shown \[ \text{[6]} \] that the
classical limit of the dynamics of quasiparticles becomes more interesting because they expe-
rience forces both from the trap and from the condensate. In the case of isotropic traps, and
hence also isotropic condensates, angular momentum conservation ensures the integrability
of the quasiparticle dynamics. This can be used to construct WKB solutions of Bogoliubov’s
wave equations for this case \[ \text{[7]} \]. In the experimentally more relevant case of axially sym-
metric traps integrability of the quasiparticle dynamics is lost and numerical studies \[ \text{[8,6]} \]
indeed have shown a generally mixed phase-space in this case. Detailed analytical work was
performed for quasiparticle energies \( E \) much smaller than the chemical potential \( \mu \). Here
two integrable limits were identified: (i) the phonon limit, where the phonon-like quasipar-
ticle is confined to the interior of the condensate and is specularly reflected back when it
strikes the surface, and (ii) a surface-particle limit, where the motion of the single-atom-like
quasiparticle consists of rapid small-amplitude oscillations between the repelling main bulk
of the condensate and the potential wall of the trap and a slow secular motion along the surface of the condensate. The numerical examination of the quasiparticle dynamics at larger energies (and for the trap anisotropy of the experiment [1]) revealed [3] a strong chaotic component at $E = \mu$ and a curious ‘quasi-integrable’ regime at $E \gg \mu$, where the dynamics in phase-space clusters around the tori corresponding to single atom motion in the trapping potential, however with small-scale chaos superimposed.

In the present paper we wish to study this large energy regime more closely, both analytically and numerically. In the spirit of Chirikov’s pioneering work on the onset of chaos (reviewed in [3]) we ask ‘where are the resonances’ and answer this question by developing the first steps of the classical perturbation theory for the quasiparticle dynamics at large energy. We also examine the influence of the thickness of the surface on the appearance of chaos. In the Thomas-Fermi approximation [3] this thickness is neglected, leading to a spatially discontinuous effective force on the quasiparticle. This violates assumptions of the KAM theorem and turns out to be the reason that noticeable small-scale chaos survives even at very large energies, where the system should be close to the integrable limit of independent atoms in the trap. Simulations with different boundary layers substantiate this hypothesis. For a condensate with boundary layer we study the transition to chaos as the energy is lowered to values comparable with the chemical potential.

II. EQUATIONS OF MOTION

In the present section we give a brief derivation of the relevant equations of motion. The starting point is the Gross-Pitaevskii equation [10]

$$i\hbar \dot{\psi}(\mathbf{x},t) = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{x}) + V_0 |\psi(\mathbf{x},t)|^2 \right\} \psi(\mathbf{x},t)$$ (2.1)

describing the macroscopic wavefunction $\psi$ of a Bose condensate at temperature $T = 0$ in a trap with potential $U$ and interaction $V_0 = 4\pi\hbar^2a/m$, where $a$ is the $s$-wave scattering length. We shall consider only the case of repulsive 2-particle interactions $a > 0$. The trap potential is taken as axially symmetric and parabolic.
\[ U(x) = \frac{m \omega_0^2}{2} (x^2 + y^2 + \lambda z^2). \] (2.2)

The ratio between axial and radial trap frequency is \( \sqrt{\lambda} \). The particle number \( N = \int d^3x |\psi(x, t)|^2 \) is conserved and assumed fixed. The equilibrium state of the condensate with chemical potential \( \mu \) is a solution of (2.1) with \( \psi(x, t) = e^{-i \mu t/\hbar} \psi_0(x) \) which satisfies

\[ \mu \psi_0(x) = \left\{ -\frac{\hbar^2 \nabla^2}{2m} + U(x) + V_0|\psi_0(x, t)|^2 \right\} \psi_0(x) \] (2.3)

with vanishing axial angular momentum

\[ L_z = \frac{i \hbar}{\hbar} \int d^3x \bar{\psi}_0(x)(x \times \nabla)\psi_0(x). \] (2.4)

The small oscillations around the equilibrium state are waves of the form

\[ \psi(x, t) = e^{-i \mu t/\hbar} (\psi_0(x) + \varphi(x, t)) \] (2.5)

with \( \varphi \) considered as small and satisfy a linearized version of eq. (2.1)

\[ i\hbar \varphi(x, t) = \left\{ -\frac{\hbar^2 \nabla^2}{2m} + U(x) - \mu + 2V_0|\psi_0(x)|^2 \right\} \varphi(x, t) + V_0 \psi_0^2(x) \varphi^*(x, t). \] (2.6)

Usually the small oscillations are considered in second quantization (where (2.6) becomes an operator equation, but retains its form), which brings out their particle-like properties, and they are then called quasiparticles. Here we shall bring out the particle properties in a different way, by considering the ‘ray-optics’ limit of eq. (2.6) [7]. Formally, this is done by means of the ansatz

\[ \varphi(x, t) = (a_0(x, t) + O(\hbar)) e^{iS(x, t)/\hbar} - (b_0(x, t) + O(\hbar)) e^{-iS(x, t)/\hbar} \] (2.7)

and considering the terms arising from eq. (2.6) formally order by order in \( \hbar \). The symmetrical form of the ansatz (2.7) allows us to restrict the sign of \( \partial S/\partial t \) by choosing \( \partial S/\partial t = -E < 0 \). \( a_0 \) and \( b_0 \) can be interpreted as semiclassical amplitudes of the quasiparticles and their antiparticles, respectively. Writing \( p = \nabla S \) for their momentum one finds to zeroth order coupled algebraic equations for the amplitudes \( a_0, b_0 \).
\[
\begin{pmatrix}
\epsilon_{HF}(x, p) + \frac{\partial S(x, t)}{\partial t} & -V_0\psi_0^2(x) \\
-V_0\psi_0^2(x) & \epsilon_{HF}(x, p) - \frac{\partial S(x, t)}{\partial t}
\end{pmatrix}
\begin{pmatrix}
a_0(x, t) \\
 b_0(x, t)
\end{pmatrix}
= 0
\] (2.8)

where
\[
\epsilon_{HF} = \frac{p^2}{2m} + U(x) - \mu + 2V_0|\psi_0(x)|^2
\] (2.9)
is called the classical Hartree-Fock energy.

Eq. (2.8) implies as solvability condition a quadratic equation for \(\partial S/\partial t\) which reduces to the Hamilton-Jacobi equation
\[
\frac{\partial S}{\partial t} + H(x, \nabla S) = 0
\] (2.10)
with
\[
H(x, p) = \sqrt{\epsilon_{HF}^2(x, p) - V_0^2|\psi_0(x)|^4}
\] (2.11)
where by the sign convention on \(\partial S/\partial t\) the positive branch of the square-root must be taken. Eqs. (2.10), (2.11) now describe the classical dynamics of the quasiparticles complementary to the waves with dynamics (2.9). The conservation of energy \(H\) and axial angular momentum \(L_z\) of the quasiparticles can be taken care off by separating
\[
S(x, t) = S_0(\rho, z) - Et - L_z\phi
\] (2.12)
where \(\rho, \phi, z\) are standard cylinder coordinates. Eq. (2.10) then reduces to
\[
H \left(\rho, z, \frac{\partial S_0}{\partial \rho}, \frac{\partial S_0}{\partial z}\right) = E
\] (2.13)
with \(|\psi_0(x)|^2 = |\psi_0(\rho, z)|^2\) and \(p^2 = p_\rho^2 + p_z^2 + L_z^2/\rho^2\) in eqs. (2.9), (2.11). Eq. (2.8) fixes only the ratio of the amplitudes \(b_0\) and \(a_0\), which, for fixed \(E\) and \(L_z\), becomes
\[
b_0 = \left[\frac{(E^2 + V_0^2|\psi_0(x)|^4)^{1/2} - E}{(E^2 + V_0^2|\psi_0(x)|^4)^{1/2} + E}\right]^{1/2} a_0
\] (2.14)
In order to determine the absolute values (apart from an arbitrary space-independent factor) one has to go to the next order in the expansion [6] where one finds as a solvability condition the conservation law.
\[
\frac{\partial}{\partial t} (|a_0|^2 - |b_0|^2) + \frac{1}{2m} \nabla \cdot (|a_0|^2 + |b_0|^2) \nabla S = 0. \tag{2.15}
\]

In the following we shall be concerned only with the classical quasiparticle dynamics described by eq. (2.13) with the Hamiltonian (2.11), (2.9).

### III. PERTURBATION THEORY FOR LARGE ENERGY

The single-particle interaction energy with the condensate is of the order of the chemical potential \( \mu \) and is only a small perturbation for energies \( E \gg \mu \). Expanding to second order the Hamiltonian takes the form

\[
H = \epsilon_0(x, p) + 2V_0|\psi_0(x)|^2 - \frac{V_0^2}{2} \frac{|\psi_0(x)|^4}{\epsilon_0(x, p)} \tag{3.1}
\]

with

\[
\epsilon_0 = \frac{p^2}{2m} + \frac{m}{2} \omega_0^2 (x^2 + y^2 + \lambda z^2) - \mu. \tag{3.2}
\]

In the following we shall restrict our discussion mainly to the case of vanishing axial angular momentum \( L_z = 0 \), but at the end we also present some results for \( L_z \neq 0 \) in order to assess to what extent the case \( L_z = 0 \) already captures the typical behaviour of the system. Experimentally modes with \( L_z = 0 \) or \( L_z \neq 0 \) can be excited depending on the symmetry of the excitation mechanism.

For \( L_z = 0 \) the dynamics is restricted to a plane containing the \( z \)-axis, which can be taken as the \( (x, z) \)-plane \( y \equiv 0, \ p_y = 0 \). The action angle variables of the unperturbed harmonic motion in the trap are

\[
x = \sqrt{\frac{2I_x}{m\omega_0}} \sin \theta_x, \quad p_x = \sqrt{2m\omega_0 I_x} \cos \theta_x
\]

\[
z = \sqrt{\frac{2I_z}{m\sqrt{\lambda}\omega_0}} \sin \theta_z, \quad p_z = \sqrt{2m\sqrt{\lambda}\omega_0 I_z} \cos \theta_z
\]

with
\[ \epsilon_0 = \omega_0 I_x + \sqrt{\lambda} \omega_0 I_z - \mu . \] (3.4)

To express the perturbed Hamiltonian in action-angle variables we need the Fourier coefficients of the condensate density and its square

\[ \bar{\rho}_{\ell n}(I_x, I_z) = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\theta_x \int_0^{2\pi} d\theta_z e^{-i(\ell \theta_x + n \theta_z)} |\psi_0(x, 0, z)|^2 \] (3.5)

\[ \bar{\rho}^2_{\ell n}(I_x, I_z) = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\theta_x \int_0^{2\pi} d\theta_z e^{-i(\ell \theta_x + n \theta_z)} |\psi_0(x, 0, z)|^4 . \]

The canonical transformation \((\theta, I) \rightarrow (\phi, J)\) with

\[ I_x = J_x - \frac{2V_0}{\omega_0} \sum_{\ell, n} \frac{\ell}{\ell + \sqrt{\lambda} n} \bar{\rho}_{\ell n}(J_x, J_z) e^{i(\ell \theta_x + n \theta_z)} \] (3.6)

\[ \phi_x = \theta_x - \frac{2V_0}{\omega_0} \sum_{\ell, n} \frac{1}{i(\ell + \sqrt{\lambda} n)} \frac{\partial \bar{\rho}_{\ell n}(J_x, J_z)}{\partial J_x} e^{i(\ell \theta_x + n \theta_z)} \]

and analogous for \(I_z, \phi_z\) removes the angle-dependence in the first order perturbation term and we are left with the second-order Hamiltonian

\[ H = \omega_0 (J_x + \sqrt{\lambda} J_z) - \mu + 2V_0 \bar{\rho}_{00}(J_x, J_z) + \frac{V_0^2}{\omega_0} \sum_{\ell, n} K_{\ell n}(J_x, J_z) e^{i(\ell \phi_x + n \phi_z)} \] (3.7)

where

\[ K_{\ell n} = -\frac{\bar{\rho}^2_{\ell n}}{2(J_x + \sqrt{\lambda} J_z) - 2\mu/\omega_0} - 4 \sum_{p, r} \left( \frac{\partial \bar{\rho}_{\ell-p,n-r}}{\partial J_x} + r \frac{\partial \bar{\rho}_{\ell-p,n-r}}{\partial J_z} \right) \frac{\bar{\rho}_{p,r}}{p + r \sqrt{\lambda}} . \] (3.8)

Eq. (3.7) differs from (3.1) only by terms of higher than second order. For irrational \(\sqrt{\lambda}\) there are no resonances to zeroth order in the interaction, but in first order isolated resonances \(\Omega_x(J_x, J_z)P + \Omega_z(J_x, J_z)R = 0\) appear with integers \(P, R\) and the perturbed frequencies

\[ \Omega_x = \omega_0 + 2V_0 \frac{\partial \bar{\rho}_{00}}{\partial J_x} \] (3.9)

\[ \Omega_z = \sqrt{\lambda} \omega_0 + 2V_0 \frac{\partial \bar{\rho}_{00}}{\partial J_z} . \]

Their distances in frequency space have to be compared with their widths, given by [9]
\[
\Delta \omega = 4 \sqrt{\frac{V_0^2 |K_{PR}(J_x, J_z)|}{\omega_0 M_{PR}(J_x, J_z)}} \tag{3.10}
\]

where
\[
\frac{1}{M_{PR}(J_x, J_z)} = \sum_{i,k=x} P_i \frac{\partial^2 \rho_{00} P_k}{\partial J_i \partial J_k} P^2_x + P^2_z, \quad P_x = P, \quad P_z = R. \tag{3.11}
\]

If resonances overlap somewhere in phase space Chirikov’s criterion \[9\] tells us that we should expect chaos there. Unfortunately, eqs. (3.7), (3.8) are too difficult to evaluate analytically for a realistic equilibrium solution \(\psi_0(x)\) of the time-independent Gross-Pitaevskii equation. However, these equations are still useful to understand some qualitative features of numerical simulations of the complete Hamiltonian dynamics at large energies.

Let us discuss in particular the case of large condensates to which the Thomas-Fermi approximation applies, in which the spatial derivative terms in eq. (2.3) are neglected. The condensate density is then given by
\[
|\psi_0(x)|^2 = \frac{\mu - (m\omega^2_0/2)(x^2 + y^2 + \lambda z^2)}{V_0} \theta(\mu - \frac{m\omega^2_0}{2}(x^2 + y^2 + \lambda z^2)). \tag{3.12}
\]

where \(\theta(x)\) is the Heaviside step-function. As \(|\psi_0(x)|^2\) is an even function of \(x, y, z\) the perturbation amplitudes are nonvanishing only for even \(\ell, n\). Therefore \(K_{PR}\) in (3.10) must be replaced by \(K_{2P2R}\). The Thomas-Fermi approximation of the condensate density (3.12) has a discontinuous first-order derivative at the surface. This means that the Fourier coefficients \(\tilde{\rho}_{\ell,n}\) and \(\tilde{\rho}^2_{\ell,n}\) at large \(|\ell|, |n|\) fall off like \(|\ell|^{-2}, |n|^{-2}\) and \(|\ell|^{-3}, |n|^{-3}\), respectively giving the \((P,R)\)-resonances for large \(|P|, |R|\) widths, which according to eq. (3.8), fall off only like \(|P|^{-1}, |R|^{-1}\). This estimate results from the second term in eq. (3.8), which is predicted to fall off only like \(|\ell|^{-2}, |n|^{-2}\). On the other hand the number of large-order resonances \(\Omega_x/\Omega_z = -R/P\) scales like \(|P|, |R|\). Therefore, barring non-generic cases where the \(|K_{PR}|\) are small for some exceptional reason, one expects large-order resonances to always overlap in the Thomas-Fermi approximation, i.e. the tori of the free harmonic oscillations in the trap will typically all be broken. By the same arguments a condensate density with \(M\) smooth derivatives and a discontinuous \(M + 1\) order derivative will give rise to resonance

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widths scaling like $|P|^{-\frac{M}{2}-1}, |R|^{-\frac{M}{2}-1}$ and tori with large $|P|, |R|$ can exist if $M > M_c = 2$.

The critical order of smoothness for general Hamiltonian systems with $f$ degrees of freedom was determined by Chirikov [9] as $M_c = 2f - 2$.

In fig. 1 a Poincaré surface of section of the dynamics at $E = 20\mu, L_z = 0$, taken at $x = 0$ and plotted in the $(\theta, I_z)$-plane is shown for the experimentally realized [1] value $\lambda = 8$. The action variable $I_z$ is plotted in units of $2\mu/\omega_0$. With the exception of tori at small $I_z$ and at large $I_z \simeq (E + \mu)/\sqrt{\lambda}\omega_0$ all tori in fig. 1 are broken. The survival of the exceptional unbroken tori can be understood from the fact that for $I_z \to 0$ or $I_x \to 0$ (with $I_z \simeq (E + \mu)/\sqrt{\lambda}\omega_0$) all the coefficients $K_{\ell,n}$ approach 0 with the exception of $K_{\ell,0}$ or $K_{0,n}$, respectively, which cannot influence appreciably tori with frequency ratios $\Omega_x/\Omega_z \simeq 8^{-1/2}$.

In fig. 1 a number of resonances with frequency ratios in the neighborhood of $\Omega_x/\Omega_z = 8^{-1/2}$ can be discerned. Their frequency ratios are given on the right hand side of the graph. To understand the position where these resonances occur we consider $\bar{\rho}_{00}$ in the Thomas-Fermi approximation

$$\bar{\rho}_{00} = \frac{4}{\pi^2 V_0} \int_0^{\pi/2} d\phi_x \int_0^{\pi/2} d\phi_z \left( \mu - \omega_0 J_x \sin^2 \phi_x - \sqrt{\lambda} \omega_0 J_z \sin^2 \phi_z \right) \theta \left( \mu - \omega_0 J_x \sin^2 \phi_x - \sqrt{\lambda} \omega_0 J_z \sin^2 \phi_z \right)$$

and evaluate the first-order frequency shifts

$$\Delta \omega_{x,z} = 2V_0 \frac{\partial \rho_{00}}{\partial J_{x,z}}$$

from the integrals

$$\Delta \omega_x = -\frac{8\omega_0}{\pi^2} \int_0^{\pi/2} d\phi_x \int_0^{\pi/2} d\phi_z \sin^2 \phi_x \theta \left( \mu - \omega_0 J_x \sin^2 \phi_x - \sqrt{\lambda} \omega_0 J_z \sin^2 \phi_z \right)$$

$$\Delta \omega_z = -\frac{8\omega_0 \sqrt{\lambda}}{\pi^2} \int_0^{\pi/2} d\phi_x \int_0^{\pi/2} d\phi_z \sin^2 \phi_z \theta \left( \mu - \omega_0 J_x \sin^2 \phi_x - \sqrt{\lambda} \omega_0 J_z \sin^2 \phi_z \right).$$

It is manifest that $\Delta \omega_{x,z}$ are negative. Near the bottom of fig. 1 the action $J_z$ is small, while $J_x \simeq (E + \mu)/\omega_0 - \sqrt{\lambda}J_z$ is large. The Heaviside function in eqs. (3.15) therefore restricts $\sin^2 \phi_x$ to small values of the order of $\mu/\omega_0 J_x = O(\mu/E)$ while $\sqrt{\lambda} \sin^2 \phi_z$ is not so restricted.
Therefore \( |\Delta \omega_x| \ll |\Delta \omega_z| \) near the bottom of fig. 1 and \( \frac{\Omega_x}{\Omega_z} - \frac{1}{\sqrt{\lambda}} \simeq \frac{\Delta \omega_x}{\sqrt{\lambda} \omega_0} - \frac{\Delta \omega_z}{\omega_0} > 0 \) holds there. In the upper parts of fig. 1 \( J_x \) is small while \( J_z \simeq (E + \mu)/\sqrt{\lambda \omega_0} - J_x/\sqrt{\lambda} \). The situation is therefore reversed and we obtain \( \frac{\Omega_x}{\Omega_z} - \frac{1}{\sqrt{\lambda}} < 0 \) by the same argument.

The periodic orbit \( z = 0, \ p_z = 0 \) which has \( J_z = 0 \) forms the lower border of the range of \( J_z \). For this case the frequency shifts \( \Delta \omega_x, \Delta \omega_z \) are easily evaluated from eq. (3.15) with the result

\[
\Delta \omega_x = -O \left( \omega_0 (\mu/\omega_0 J_x)^{3/2} \right) \]

(3.16)

\[
\Delta \omega_z = -\frac{2}{\pi} \sqrt{\frac{\lambda \omega_0 \mu}{J_x}}
\]

indicating that the fixed point is stable for \( E \gg \mu \). The arguments of the previous paragraph indicate, furthermore, that \( |\Delta \omega_x| \) is minimal for this case, while \( |\Delta \omega_z| \) is maximal, leading to a maximal value of the ratio

\[
\left( \frac{\Omega_x}{\Omega_z} \right)_{\text{max}} \simeq \frac{1}{\sqrt{\lambda}} + \frac{2}{\pi} \sqrt{\frac{\mu}{\lambda \omega_0 J_x}} \simeq \frac{1}{\sqrt{\lambda}} \left( 1 + \frac{2}{\pi} \sqrt{\frac{\mu}{E + \mu}} \right)
\]

(3.17)

where we used \( E + \mu \simeq \omega_0 J_x + \sqrt{\lambda \omega_0} J_z \) with \( J_z = 0 \) in the last estimate. For \( E/\mu = 20 \) this gives \( (\Omega_x/\Omega_z) \simeq 0.402 \), which is just barely larger than the ratio 0.4 of the 2:5 resonance visible near the lower border of fig. 1. Similar arguments apply to the upper border of the range of \( J_z \) which is formed by the periodic orbit \( x = 0, \ p_x = 0 \) with vanishing \( J_x \) for which

\[
\Delta \omega_x = -\frac{2}{\pi} \sqrt{\frac{\omega_0 \mu}{\sqrt{\lambda} J_z}} , \quad \Delta \omega_z = -\sqrt{\lambda \omega_0} O \left( (\mu/\sqrt{\lambda} \omega_0 J_z)^{3/2} \right) .
\]

(3.18)

Thus

\[
\left( \frac{\Omega_x}{\Omega_z} \right)_{\text{min}} \simeq \frac{1}{\sqrt{\lambda}} \left( 1 - \frac{2}{\pi} \sqrt{\frac{\mu}{E + \mu}} \right) .
\]

(3.19)

For \( E/\mu = 20 \) this yields \( (\Omega_x/\Omega_z)_{\text{min}} \simeq 0.304 \) which is smaller than the ratio 0.333 of the 1:3 resonance visible near the upper border of fig. 1.

In general we can conclude that for fixed energy \( E \) we should expect to see the strongest resonances in the interval
\[
\frac{1}{\sqrt{\lambda}} \left( 1 - \frac{2}{\pi} \sqrt{\frac{\mu}{E + \mu}} \right) < \Omega_x/\Omega_z < \frac{1}{\sqrt{\lambda}} \left( 1 + \frac{2}{\pi} \sqrt{\frac{\mu}{E + \mu}} \right), \tag{3.20}
\]

which are, for \( \lambda = 8 \), \( E/\mu = 20 \), the resonances 1:3, 2:5, 3:8, 4:11, 5:14, 6:17 and are indeed all seen in fig. 1 with the exception of the 5:14 resonance. In its place a chaotic region is seen.

The resonance values of the actions following from the perturbation theory are indicated on the right-hand side of fig.1. The 4:11 resonance predicted close to the missing 5:14 resonance is nearly completely destroyed and barely separated from the chaotic region replacing the 5:14 resonance.

Let us now consider the effect of the sharpness of the boundary layer of the condensate. Its thickness is given by the healing length \[ \ell_H = \frac{\hbar}{\sqrt{2m\mu}}. \tag{3.21} \]

It enters as an independent parameter whose ratio to the radial Thomas-Fermi radius \( \rho_{TF} = \sqrt{2\mu/m\omega_0^2} \) is determined by the value of the chemical potential, i.e. by the number of particles in the trap, \( \ell_H/\rho_{TF} = \hbar\omega_0/2\mu \). As example we consider \( \ell_H/\rho_{TF} = 0.1 \). The condensate with boundary layer is modelled by joining

\[
|\psi_0(x)|^2 = \frac{\mu - \frac{1}{2}m\omega_0^2r^2}{V_0} \theta(\rho_{TF} - \ell_H - r)
+ \exp(-a_0 - a_1(r - \rho_{TF} + \ell_H) - a_2(r - \rho_{TF} + \ell_H)^2 \\
- a_3(r - \rho_{TF} + \ell_H)^3) \theta(r - \rho_{TF} + \ell_H)
\]

continuously with continuous three derivatives at \( r = \rho_{TF} - \ell_H \), thereby fixing \( a_0, \ldots, a_3 \).

Here the abbreviation \( r = \sqrt{\rho^2 + \lambda z^2} \) is used. The degree of smoothness thereby introduced should be sufficient to see smooth KAM tori. The model condensate (3.22) is of course not a solution of the Gross-Pitaevskii equation, but does not differ qualitatively from solutions taking into account the boundary layer [11]. For our present purposes it is therefore perfectly acceptable while avoiding unnecessary complications. In fig. 2 we compare Poincaré surface of sections in the same format as in fig.1 for the Thomas-Fermi approximation and the smooth model condensate with \( l_H/\rho_{TF} = 0.1 \) at energy \( E/\mu = 100 \) and \( \lambda = 8 \). It
can be seen that with the smooth boundary layer included most of the broken tori of the Thomas-Fermi condensate seen in the upper part of fig.2 become smooth, as seen in the lower part of fig.2, however with ripples on the tori still indicating the presence of the narrow boundary layer. If the boundary layer is narrowed further (not shown) these ripples become stronger and develop sharp cusps. The chaotic band at small actions \( I_z \) survives even for very large quasiparticle energies \( E/\mu \). Resonances within this band have a comparatively large width for two reasons. For one the factors \( 1/M_{PR} \) are large, because \( I_z \) is not far above the value \( I_z = \mu/\omega_0 \sqrt{\lambda} \) where \( M_{PR}^{-1} \) peaks (with a logarithmic singularity in Thomas-Fermi approximation). For larger values of \( I_z \), of the order of \( E/\omega_0 \sqrt{\lambda} \), like for the 6:17 resonance or values of \( P : R \) close to \( \sqrt{\lambda} \), \( 1/M_{PR} \) is much smaller by a factor of the order of \((\mu/E)^2\). Second, the interaction coefficient \( |K_{PR}| \) has a resonantly enhanced contribution \(-4(\partial \bar{\rho}_{00}/\partial J_z) \bar{\rho}_{2P2R}(P/R + \sqrt{\lambda})^{-1}\). The last factor in this expression favors resonances \( P : R \) close to the ratio \( \sqrt{\lambda} \). The existence of the narrow boundary layer of the condensate furthermore leads to appreciable interaction coefficients \( |K_{PR}| \) even for comparatively high-order resonances whose overlap may be responsible for the formation of the chaotic band. The requirement that both factors \( M_{PR}^{-1} \) and \( |K_{2P2R}| \) must be large may explain the appearance of a band of actions \( I_z \) with appreciable resonance overlap somewhat above the value \( I_z = \mu/\omega_0 \sqrt{\lambda} \).

Dynamically the chaotic band is related to orbits in a layer of actions \( I_z \gtrsim \mu/\sqrt{\lambda}/\omega_0 \) which are just sufficient for the quasiparticle to hit or miss the condensate at random as it oscillates back and forth in x-direction. This mechanism is able to introduce sensitive dependence on initial conditions and exists, if only in a narrow band, even at very large energies. For just slightly smaller actions \( I_z \) the quasiparticle has to pass the condensate twice in each period of \( \theta_x \) and the tori are smooth even in Thomas-Fermi approximation, as can be seen in fig. 1 for \( E/\mu = 20 \). A similar mechanism for a chaotic band should actually exist also for the oscillations in the z-direction, the short axis of the condensate-ellipsoid. However the instability in this case for action \( I_z \gtrsim \mu/\sqrt{\lambda}/\omega_0 \) seems to be much less pronounced (which is plausible, because the perturbation by the condensate should be
weaker along the short axis) and is not visible in the numerical data.

Finally we consider numerically the transition to chaos in the condensate with boundary layer \( l_H/\rho_{TF} = 0.1 \) as the quasiparticle energy is lowered. In fig.3 the same Poincaré surface of section is plotted as in figs.1,2 (and again for \( \lambda = 8 \)) but in the \((z, p_z)\)-plane rather than the \((\theta, I_z)\)-plane. The two plots in the upper row are for \( E/\mu = 100 \) and \( E/\mu = 20 \), those in the lower row are for \( E = 10 \) and \( E = 2 \) respectively. The plots for \( E = 100 \) and \( E = 20 \) can be compared with fig.2 and fig.1 respectively, but fig.1 is, of course for vanishing \( l_H \) only. The slightly rounded Thomas-Fermi surface at \( z/\rho_{TF} = \lambda^{-1/2} \) is visible in these graphs.

Based on these and similar plots the transition to chaos can now be roughly described as follows: The chaotic band in a layer of small actions \( I_z \gtrsim \mu/\sqrt{\lambda \omega_0} \) existing even at very large energies (see the plot for \( E/\mu = 100 \)) becomes wider as the energy is lowered (see \( E/\mu = 20 \)). Then, at a critical energy \( E/\mu = 13.9 \) which we discuss further below, the periodic orbit along the long axis of the condensate-ellipsoid becomes unstable and a second chaotic region in phase-space surrounding the unstable orbit \( z = 0 = p_z \) is created. The inner and outer chaotic regions then rapidly grow together as the energy is lowered further (see \( E/\mu = 10 \)) and finally fill up most of the accessible regions of phase-space (see the last plot with \( E/\mu = 2 \)).

Apart from a continuous widening of the chaotic regions the main event in this transition to chaos is the appearance of the instability of the periodic orbit along the long axis of the condensate-ellipsoid, which for \( \lambda > 0 \) is the \( x \)-axis. In Thomas-Fermi approximation this orbit has the time-dependence for \( |x| < \rho_{TF} \)

\[
x = \rho_{TF} \sqrt{E/\mu - 1} \sinh(\omega_0 t - \varphi^o)
\]

(3.23)

\[
p_x = m\omega_0 \rho_{TF} \sqrt{E/\mu - 1} \cosh(\omega_0 t - \varphi^o)
\]

and for \( |x| > \rho_{TF} \)

\[
x = \rho_{TF} \sqrt{E/\mu + 1} \sin(\omega_0 t - \varphi^o)
\]
with $\varphi^o$ and $\varphi'^o$ suitably adjusted by continuity at $|x| = \rho_{TF}$. To determine the energy where this orbit looses its stability we can perform a linear stability analysis for small perturbations $z, p_z$ away from this orbit, which satisfy

$$m \dot{z} = p_z, \quad \dot{p}_z = \lambda \left(1 - 2\theta(|x(t)| - \rho_{TF}) \right) m \omega_0^2 z.$$ \hspace{1cm} (3.25)

The growth of a perturbation of the periodic orbit is determined by the monodromy matrix $M$ for a half-period $T/2$

$$
\begin{pmatrix}
    z(T/2)/\rho_{TF} \\
    p_z(T/2)/m \omega_0 \rho_{TF}
\end{pmatrix} =
M
\begin{pmatrix}
    z(0)/\rho_{TF} \\
    p_z(0)/m \omega_0 \rho_{TF}
\end{pmatrix}.
$$ \hspace{1cm} (3.26)

The Hamiltonian form of the dynamics ensures that $\text{Det} \ M = 1$. The stability condition for the perturbations in $z$-direction then becomes

$$|\text{Tr} M| \leq 2.$$ \hspace{1cm} (3.27)

With a little algebra it is straight-forward to evaluate $M$ and its trace thereby reducing (3.27) to

$$|\cos (\sqrt{\lambda} \omega_0 t_2) \cosh (\sqrt{\lambda} \omega_0 t_1)| \leq 1$$ \hspace{1cm} (3.28)

Here $t_1$ and $t_2$ are the total lengths of the time-intervals during each half-period where $|x| < \rho_{TF}$ and $|x| > \rho_{TF}$, respectively. They are given by

$$t_1 = \frac{2}{\omega_0} \text{Artanh} \sqrt{\frac{\mu}{E}}, \quad t_2 = \frac{2}{\omega_0} \text{Arctan} \sqrt{\frac{E}{\mu}}.$$ \hspace{1cm} (3.29)

For $\lambda = 8$ stability is lost, according to the criterion (3.28) for $E/\mu = 14.4$ which is in reasonable agreement with the already quoted value $E/\mu = 13.9$ determined from the numerical simulation of the complete quasiparticle dynamics.
IV. CONCLUSION

In the present paper we have studied the classical limit of the dynamics of the quasiparticles in a spatially inhomogeneous harmonically trapped weakly interacting Bose gas. As is well known many properties of a Bose gas are determined by its quasiparticles. For sufficiently large energies $E/\hbar \omega_0 \gg 1$ a classical description of quasiparticles should be possible. We have accordingly concentrated our attention on the large energy regime. For quasiparticle energies large compared to the chemical potential a perturbative expansion becomes possible. The dynamics then looks like that of an anisotropic harmonically bound particle which is perturbed by the presence of a weakly repelling condensate localized around the center of the trap with a rather sharp surface. The appearance of an infinitely sharp surface in the Thomas-Fermi approximation leads to the break-up of all tori with the exception of those in the immediate phase-space neighborhood of the periodic orbits along the main axes of the ellipsoidal condensate. Therefore in this case chaos exists in phase-space for arbitrarily large energies $E/\mu$. Still resonances can be identified even in this case and their actions are well described by perturbation theory. We have compared this non-smooth case to that of a condensate with a smooth (up to third derivatives) but narrow boundary layer. In real condensates the thickness of the boundary layer is determined by the two-particle interaction and the number of particles \[15\]. In that case smooth KAM tori exist at sufficiently large energies, but they are rippled by the influence of the boundary layer. Furthermore it turns out that an appreciable region of chaos in phase-space persists even to large energies. It is related to orbits along the long axis of the condensate-ellipsoid which are sufficiently perturbed in the direction of the short axis to sometimes miss and sometimes hit the condensate in a random way with sensitive dependence on small perturbations. Finally we have studied how large scale chaos appears as the energy is gradually lowered to values of the order of the chemical potential. The instability of the periodic orbit along the long axis of the ellipsoid was found to play a major role in this transition. It is connected with the appearance of a second inner chaotic region at lower energies which joins up with the chaotic...
band existing also at large energies.

Our discussion so far has been restricted to the special case $L_z = 0$, where the classical quasiparticle dynamics is confined to a plane in configuration space containing the $z$-axis. One may well ask to what extent this motion already captures the typical behavior of the system. To examine this question at least numerically we have generated Poincaré surface of sections for $L_z \neq 0$ both for fixed $E$ and varying $L_z$ or for fixed $L_z$ and varying $E$. The surfaces of section are always taken at the value $\rho = \rho_0$ where the effective potential in radial direction, which includes the centrifugal barrier, has its minimum. In fig.4 we present a series of Poincaré surfaces of sections for $L_z$ fixed at a rather high value (in units of $\hbar$) $L_z = \mu/\omega_0$ and the same values of $E$ and also the same thickness of the boundary layer as in fig.3.

It is apparent that taking $L_z \neq 0$ the mirror symmetry with respect to the $z$-axis and the $p_z$-axis which is present at $L_z = 0$ is lost and replaced by a point symmetry with respect to the origin $z = p_z = 0$, which is, of course, to be expected. However, apart from this obvious difference the qualitative behavior displayed in fig.4 is the same as in fig.3. As was shown in [6] the energy and the angular momentum must satisfy the inequalities

$$E + \mu > \omega_0 L_z \quad \text{if} \quad E > \mu$$

$$E > (\omega_0 L_z)^2/4\mu \quad \text{if} \quad E < \mu.$$  

(4.1)

For $E > \mu$ and $|L_z| > 2\mu/\omega_0$ there exists a domain $(\omega_0 L_z)^2/4\mu > E > \omega_0 L_z - \mu$ where the motion of the quasiparticles occurs outside the condensate in the Thomas-Fermi limit, and is therefore integrable. Thus an additional transition from nonintegrable to integrable dynamics occurs for very high angular momentum $|L_z| > 2\mu/\omega_0$ as the energy is lowered from above to below $E = (\omega_0 L_z)^2/4\mu$.

Let us finally turn to the quantum mechanical implications of the classical dynamics we have studied. Such implications exist both for the wavefunctions and the energies of single quasiparticle states which are of course closely connected. As the classical analysis is done in phase space it is most convenient for a discussion to use the Husimi distribu-
tion \( Q(\rho, p_\rho, z, p_z) = | < \alpha | \psi > |^2 \) where \( | \alpha > \) is a coherent state of the harmonic oscillators defined by the free trap. For each quantum state \( | \psi > \) the function \( Q \) is a positive quasiprobability on the phase space, which due to the overcompleteness of the \( | \alpha > \), contains the full information on \( | \psi > \).

Let us now turn to the Poincaré surface of sections displayed in fig.3 and discuss the corresponding quantum states via their \( Q \)-functions: In fig.3a the \( Q \)-functions at \( \rho = 0 \) will be spread out along the tori with (in the limit \( \hbar \omega_0/\mu \to 0 \)) narrow peaks on the tori. The number of such states is semiclassically given by the phase space volume of the energy shell of thickness \( \Delta E \) in units \( (2\pi \hbar)^2 \). The chaotic layer visible in fig.3a may correspond to several quantum states (depending on the contribution of this layer to the phase space volume of the energy shell in units \( (2\pi \hbar)^2 \)) which are all spread out along the layer but with wave functions oscillating wildly in the corresponding configuration space so as to satisfy the orthogonality condition. If indeed several such states exist in an energy shell of thickness \( \Delta E \) their energies will tend to repell each other. The energies corresponding to \( Q \)-functions centered on tori will show no such repulsion.

Essentially the same discussion applies to fig.3b, 3c where the chaotic layer occupies a larger fraction of the phase-space volume and finally merges into a single domain. In the case of fig.3d, where essentially a single chaotic domain survives two different types of quantum states are possible: The first possibility is that the quantum states are all spread out over the chaotic domain with strong oscillations of their wave functions in the corresponding domain of configuration space to satisfy orthogonality and accompanying strong level repulsion. The second possibility is that the quantum states show dynamical localization with respect to the action variable \( I_z \). In this case the quantum states still localize around different values of \( I_z \) due to a coherent interference effect akin to Anderson localization. In this case the wave functions can be orthogonal without energy level repulsion. Which of these two possibilities is realized depends on the strength of the chaotic change of the action variable \( I_z \). If this change is sufficiently large, then the first possibility (extended states with level repulsion) will be realized. If however \( I_z \) changes sufficiently weakly in a diffusive way such that its
variance satisfies $< \Delta I_z^2 > = Dt$ with a diffusion constant $D$, then the second possibility may be realized. Then a fundamental estimate [13] can be made of the localization length $\xi_z$ of $I_z$ according to $\xi_z^2 \sim D\rho(E)$ where $\rho(E)$ is the density of states at energy $E$. Dynamical localization then is predicted to occur as soon as $\xi_z \ll W_z$ where $W_z$ gives the width of the chaotic domain in $I_z$. Thus $D \ll W_z^2/\hbar \rho(E)$ is required. At present no reliable estimate of $D$ exists, either analytically or numerically, so the question which of the two behaviors will occur in a given trap at energies $E \sim \mu$ must be left open here. Numerical computations of quasiparticle energies have been performed for certain trap parameters and avoided crossings have been seen in the results for the regime $E \sim \mu$ (see e.g. [12]), but a systematic study of the level statistics has not yet been performed for this case.

However, the level repulsion typical for classically chaotic systems has already been built into a quantum theory of damping of the low-energy collective modes due to scattering of thermally excited quasiparticles at energies of the order of the chemical potential [14]. This should only be a beginning. If the precedence of mesoscopic systems is any hint, we may expect that more properties of trapped Bose condensates will turn out to be infiltrated by chaos in the future.

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FIGURE CAPTIONS

Fig. 1. Poincaré surface of section of the quasiparticle dynamics. The cut is taken at constant energy at $x = 0, \ p_x > 0$ for energy $E/\mu = 20$ and $\lambda = 8$. The cross-section is presented in the $(\theta_z, I_z)$-plane, where $\sqrt{\lambda}\omega_0 I_z = p_z^2/2m + (m\lambda\omega_0^2/2)z^2$, $\arctan \theta_z = m\sqrt{\lambda}\omega_0 z/p_z$. The
action variable $I_z$ is given in units of $2\mu/\omega_0$. Frequency ratios $\Omega_x : \Omega_z$ of resonances are given on the right hand margin together with the resonance actions determined from perturbation theory. For resonances existing in doublets related by symmetries only one member of the doublet is shown for clarity. The 5:14 resonance could not be detected numerically.

**Fig. 2.** Poincaré surface of sections as in fig.1 for $E/\mu = 100$ for the dynamics with the condensate in Thomas-Fermi approximation (upper part) and for the condensate with boundary layer of thickness $l_H/\rho_{TF} = 0.1$, continuous up to and including the third derivative (lower part).

**Fig. 3.** Poincaré surface of sections as in figs.1,2 but plotted in the $(z, p_z)$-plane. $z, p_z$ are plotted in units $\sqrt{2\mu/m\omega_0^2}, \sqrt{2m\mu}$. The value of $E/\mu$ is 100 (upper left), 20 (upper right), 10 (lower left), and 2 (lower right).

**Fig. 4.** Poincaré surface of sections as in fig.3, but for finite angular momentum $L_z = \mu/\omega_0$. Again the values of $E/\mu$ are 100 (upper left), 20 (upper right), 10 (lower left), and 2 (lower right).
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