Classical quasi-particle dynamics in trapped Bose condensates

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(June 14, 2021)

The dynamics of quasi-particles in repulsive Bose condensates in a harmonic trap is studied in the classical limit. In isotropic traps the classical motion is integrable and separable in spherical coordinates. In anisotropic traps the classical dynamics is found, in general, to be nonintegrable. For quasi-particle energies $E$ much smaller than the chemical potential $\mu$, besides the conserved quasi-particle energy, we identify two additional nearly conserved phase-space functions. These render the dynamics inside the condensate (collective dynamics) integrable asymptotically for $E/\mu \to 0$. However, there coexists at the same energy a dynamics confined to the surface of the condensate, which is governed by a classical Hartree-Fock Hamiltonian. We find that also this dynamics becomes integrable for $E/\mu \to 0$ because of the appearance of an adiabatic invariant. For $E/\mu$ of order 1 a large portion of the phase-space supports chaotic motion, both, for the Bogoliubov Hamiltonian and its Hartree-Fock approximant. To exemplify this we exhibit Poincaré surface of sections for harmonic traps with the cylindrical symmetry and anisotropy found in TOP traps. For $E/\mu \gg 1$ the dynamics is again governed by the Hartree-Fock Hamiltonian. In the case with cylindrical symmetry it becomes quasi-integrable because the remaining small chaotic components in phase space are tightly confined by tori.

03.75-Fi, 67.40.Db, 03.65Sq

I. INTRODUCTION

The experimental realization of Bose-condensates of atoms harmonically bound in magnetic traps \[1,2\] call for a space-dependent version of Bogoliubov’s theory, or some modification thereof. Such a theory proceeds by splitting the field operator $\hat{\psi}(\mathbf{x})$ and its adjoint in a $C$-number part $\psi_0(\mathbf{x})$ and a residual operator $\hat{\varphi}(\mathbf{x})$,

$$\hat{\psi}(\mathbf{x}) = \psi_0(\mathbf{x}) + \hat{\varphi}(\mathbf{x}) \quad (1)$$

and an accompanying decomposition of the Hamiltonian in terms of 0, 1, 2, 3, 4 order in $\varphi, \varphi^+$. The term of 1 order in $\varphi, \varphi^+$ is made to vanish by choosing $\psi_0(\mathbf{x})$ to satisfy the time-independent Gross-Pitaevskii equation \[4\], which at low temperatures, takes the form

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_0(\mathbf{x}) + (U(\mathbf{x}) - \mu) \psi_0(\mathbf{x}) + V_0 |\psi_0(\mathbf{x})|^2 \psi_0(\mathbf{x}) = 0 \quad (2)$$

with the normalization $\int |\psi_0|^2 d^3x = N_0$. Here

$$U(\mathbf{x}) = \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \quad (3)$$

is the generally anisotropic harmonic trap potential,
\( V_0 = \frac{4\pi\hbar^2 a}{m} \) (4)

is the strength of the pseudo-potential replacing the true two-particle potential at low energies, with the s-wave scattering length \( a \), which is here assumed to be positive.

For \((N_0 a / d_0) \gg 1\), where \( d_0 = \sqrt{\hbar/\omega} \), \( \omega = (\omega_x \omega_y \omega_z)^{1/3} \), the solution to the Gross-Pitaevskii equation can be determined in the Thomas-Fermi approximation [5] by neglecting the kinetic-energy term

\[
|\psi_0|^2 = \frac{\mu - U(x)}{V_0} \Theta(\mu - U(x)).
\] (5)

In the following we shall choose \( \psi_0 \) as real and positive. The chemical potential is determined from the normalization. The next step is the diagonalization of that part of \( H \), which is a quadratic form in \( \hat{\phi}, \hat{\phi}^+ \), by a Bogoliubov transformation

\[
\hat{\phi}(x) = \sum_j (U_j(x) \hat{\alpha}_j - V_j^*(x) \hat{\alpha}_j^+)
\] (6)

with

\[
\int d^3x (|U_j(x)|^2 - |V_j(x)|^2) = 1
\] (7)

and

\[
[\alpha_j, \alpha_{j'}] = 0 = [\alpha_j^+, \alpha_{j'}^+]
\]

\[
[\alpha_j, \alpha_{j'}^+] = \delta_{jj'}.
\] (8)

The second-order part of \( H \) is diagonalized by this transformation, if \( U_j(x) \) and \( V_j(x) \) satisfy the Bogoliubov equations

\[
\left( \begin{array}{cc}
\hat{H}_{HF} & -K(x) \\
-K(x) & \hat{H}_{HF}
\end{array} \right) \left( \begin{array}{c}
U_j \\
V_j
\end{array} \right) = E_j \left( \begin{array}{c}
U_j \\
V_j
\end{array} \right)
\] (9)

with the Hartree-Fock Hamiltonian

\[ \hat{H}_{HF} = -\frac{\hbar^2}{2m} \nabla^2 + U(x) - \mu + 2V_0|\psi_0(x)|^2 \] (10)

and the coupling term

\[ K(x) = V_0|\psi_0(x)|^2 \] (11)

between the two components \( U_j(x), V_j(x) \) of a quasi-particle wave-function. Because of the different signs of the \( U_j, V_j \) components on the right-hand side, they play the role of particle and anti-particle components of the complete wave-function. As the equations are symmetric under the particle-antiparticle transformation \( E_j \rightarrow -E_j, U_j \rightarrow V_j^*, V_j \rightarrow U_j^* \) we may define \( E_j \) to be non-negative without restriction of generality. Various numerical [6] and approximate analytical [7] treatments of these equations are available in the literature.

In the present paper we wish to study the classical limit of the center-of-mass motion of the quasi-particles. In order to discuss the dynamics rather than the eigenstates of the quasi-particles, it is useful to introduce time-dependent wave functions via

\[
\left( \begin{array}{c}
U(t) \\
V(t)
\end{array} \right) = \sum_j c_j \left( \begin{array}{c}
U_j \\
V_j
\end{array} \right) e^{-iE_j t/\hbar}
\] (12)

with arbitrary coefficients \( c_j \). They satisfy the time-dependent Schrödinger equation

\[
i\hbar \frac{\partial}{\partial t} \left( \begin{array}{c}
U(t) \\
-V(t)
\end{array} \right) = \left( \begin{array}{cc}
\hat{H}_{HF} & -K \\
-K & \hat{H}_{HF}
\end{array} \right) \left( \begin{array}{c}
U(t) \\
V(t)
\end{array} \right).
\] (13)
For large energies $E_j$, $E_j \gg \mu$, the classical motion can be interpreted as the center of mass-motion of quasi-particle wave packets. For small energies $E_j$, $E_j \ll \mu$, such a straightforward physical interpretation of the classical quasi-particle dynamics is no longer possible. However, even in this regime, there is still a close mathematical relation between the classical and the quantum dynamics, as the classical trajectories are the characteristics of the quantum mechanical wave-equation. This is made explicit by the derivation of the classical dynamics as a limit of the Schrödinger equation via the Hamilton-Jacobi equation. The Hamilton-Jacobi equation corresponding to eq. (13) is obtained by the asymptotic ansatz for $\hbar \to 0$
\[
\left( \begin{array}{c} U(x,t) \\ V(x,t) \end{array} \right) \simeq \left( \begin{array}{c} a_0(x,t) + 0(\hbar) \\ b_0(x,t) + 0(\hbar) \end{array} \right) e^{iS(x,t)/\hbar}
\]
with $\int d^3x (|a_0(x,t)|^2 - |b_0(x,t)|^2) = 1$. It reduces eq. (13) to the form, to zeroth order in $\hbar$,
\[
\left( \begin{array}{cc} \epsilon_{HF} + \frac{\partial S}{\partial t} & \epsilon_{HF} - \frac{\partial S}{\partial t} \\ -K & -K \end{array} \right) \left( \begin{array}{c} a_0 \\ b_0 \end{array} \right) = 0.
\]
Here
\[
\epsilon_{HF} = \frac{p^2}{2m} + U(x) - \mu + 2V_0|\psi_0(x)|^2.
\]
We may restrict to $-E = \partial S/\partial t \leq 0$ in accordance with our restriction on $E$. To first order in $\hbar$ we obtain
\[
\frac{\partial}{\partial t} \left( \begin{array}{c} a_0 \\ -b_0 \end{array} \right) + \frac{1}{2m} \nabla \cdot \left( (\nabla S) \left( \begin{array}{c} a_0 \\ b_0 \end{array} \right) \right) + \frac{1}{2m} \nabla S \cdot \nabla \left( \begin{array}{c} a_0 \\ b_0 \end{array} \right) = \frac{i}{\hbar} \left( \begin{array}{cc} \epsilon_{HF} + \frac{\partial S}{\partial t} & \epsilon_{HF} - \frac{\partial S}{\partial t} \\ -K & -K \end{array} \right) \left( \begin{array}{c} a_1 \\ b_1 \end{array} \right)
\]
Here $(a_0, b_0)$ are the $0(\hbar)$-components of the amplitudes in (14). These will exist, and the expansion will be well-defined, only if the left-hand side of (17) is orthogonal on the kernel $(a_0, b_0)$ of the matrix in (15), which also appears on the right-hand side of (17). This condition gives rise to the conservation law
\[
\frac{\partial}{\partial t}(|a_0|^2 - |b_0|^2) + \frac{1}{2m} \nabla \cdot ((|a_0|^2 + |b_0|^2)\nabla S) = 0
\]
which ensures that the normalization condition
\[
\int d^3x (|a_0|^2 - |b_0|^2) = 1
\]
is consistent with the classical dynamics and represents the classical limit of the continuity equation following from (13) [8]. The zeroth order equation has a nontrivial solution only if the determinant condition
\[
\left( \frac{\partial S}{\partial t} \right)^2 = \epsilon_{HF} - K^2
\]
is satisfied, which, observing our sign convention for $\partial S/\partial t$, gives the time-dependent Hamilton-Jacobi equation
\[
\frac{\partial S(x,t)}{\partial t} + H \left( x, \frac{\partial S}{\partial x} \right) = 0
\]
with the classical Hamiltonian
\[
H(x,p) = \sqrt{\epsilon_{HF}(x,p) - K(x)^2}.
\]
The time-independent Hamilton Jacobi equation results from the separation
\[
S(x,t) = S(x) - Et
\]
and reads
\[
H(x, \frac{\partial S}{\partial x}) = E.
\]
If we can neglect the $0(\hbar)$-corrections $a_i, b_i$ in (12) we obtain from the first order equation separate conservation laws for the quasi-particle and anti-quasi-particle densities

\[
\frac{\partial}{\partial t} |a_0(x,t)|^2 + \frac{1}{2m} \nabla \cdot ((|a_0(x,t)|^2 \nabla S) = 0 \\
\frac{\partial}{\partial t} |b_0(x,t)|^2 - \frac{1}{2m} \nabla \cdot ((|b_0(x,t)|^2 \nabla S) = 0.
\]

The classical antiparticle and particle dynamics are therefore just the time-reversed of each other, and the densities of both components are separately conserved.

In the following sections we analyze the classical dynamics described by the Hamiltonian (23).

\section{II. Classical Quasi-Particle Dynamics}

For the case of isotropic harmonic traps angular momentum is conserved and the quasi-particle dynamics is integrable and separable in spherical coordinates. This case is discussed in [1], where it is made the basis of a semiclassical quantization procedure. Therefore, in the following we concentrate on the analysis of the case of anisotropic harmonic traps in the limit where the Thomas-Fermi approximation applies. In the present section we shall assume cylindrical symmetry of the trap

\[ U(x) = \frac{m\omega_0^2}{2}(x^2 + y^2) + \frac{m\omega_z^2}{2}z^2 \]

In the experiment \[ \omega_z > \omega_0, \] namely, \((\omega_z/\omega_0)^2 \approx 8\). As the parameter denoting the anisotropy of the potential we introduce \( \epsilon \) by \( \epsilon^2 = 1 - (\omega_0/\omega_z)^2 \), which is the numerical eccentricity of the Thomas-Fermi surface \( \mu = U(x) \), a rotational symmetric ellipsoid. This two-dimensional surface is the boundary of the condensate.

Our problem has a characteristic energy, namely the chemical potential. Thus, the second relevant parameter of the classical motion is the ratio \( E/\mu \). We note that measuring the energy in units of \( \mu \), coordinates, momenta and time in units of

\[ r_0 = \sqrt{\frac{2\mu}{m\omega_0^2}}, \quad p_0 = \sqrt{2m\mu}, \quad t_0 = \omega_0^{-1} \]

respectively, the dimensionless Hamiltonian can be put in a form, which depends only on the anisotropy parameter \( \epsilon \). This shows that condensates with the same anisotropy but with different chemical potential behave similarly in the classical description, if the physical quantities are scaled appropriately.

In the isotropic case \( \epsilon = 0 \) the classical dynamics are completely integrable. As three independent constants of motion we can choose the energy \( E \), the modulus of the angular momentum and its \( z \)-component \( L_z \). As we keep rotational symmetry around the \( z \)-axis in the anisotropic case \( \epsilon \neq 0 \) the \( L_z \) and of course the energy are still conserved quantities, whereas the total angular momentum considered here is no longer a constant of motion. Thus, in the following we shall investigate the classical behaviour of this three degrees of freedom system depending on the two constants of motion \( E \) and \( L_z \), and we address the question whether the dynamics are integrable or chaotic.

Let us introduce the usual cylindrical coordinates \( \rho = \sqrt{x^2 + y^2}, z \) and \( \phi \). Because of the rotational symmetry around of the \( z \)-axes the angle \( \phi \) is a cyclic variable. In cylindrical variables the Hamiltonian has merely two degrees of freedom \( \rho \) and \( z \), \( L_z \) just enters as a parameter. Certain conditions have to be satisfied as can be seen from the Hamiltonian in the region outside the condensate. For \( E > \mu \) the condition \( E + \mu > \omega_0 L_z \) has to be guaranteed, for \( E < \mu \) we must have \( E > (\omega_0 L_z)^2/4\mu \).

The dynamics of this twodimensional system we can visualize by Poincaré cuts, see Fig.\[ . \] For different energies we observe different dynamical behaviour. For \( E > (\omega_0 L_z)^2/4\mu \) two different kinds of trajectories can occur typically. If the repulsive effective potential in \( \rho \)-direction due to the angular momentum \( L_z \) is strong enough, the particle cannot enter the condensate and is only moving in the harmonic potential of the external trap. The motion in an anisotropic harmonic potential is completely integrable, as a third constant of motion we can choose the energy in the \( z \)-degree of freedom \( E_z = p_z^2/2m + m\omega_z z^2/2 \). These trajectories, which are not perturbed by the condensate, can be seen as the integrable tori around the fixed point of the Poincaré map in the centre of Fig.\[ . \] which is the periodic orbit moving only in \( z \) and \( \phi \) directions. If the particle enters the condensate, \( E_z \) is no more a conserved quantity. Nevertheless for energies large compared to the chemical potential also those trajectories are still quite similar to unperturbed motion. Typically the trajectories are confined to thin stochastic layers separated by each other by
integrable tori. No Arnold diffusion occurs, as usually for a system of two, not of three degrees of freedom. At high energies the system behaves quasi integrable. The influence of the condensate can be taken as a small perturbation to the motion in the external potential.

For energies in the range $10 > E/\mu > 0.1$ (Fig. 2) we typically observe a mixed phase space. The fixed point is now inside the condensate, but does not loose its stability. The detailed structure depends on the parameters chosen. Already for small anisotropy ($\epsilon^2 = 0.2$) a relevant part of phase space can be chaotic. This shows that for energies of the order of the chemical potential the isotropic case with its integrable dynamics is an exceptional rather than a typical situation. If $E < \mu$ all trajectories move inside and outside the condensate.

For energies small compared to the chemical potential $E < 0.1\mu$ (Fig. 3) the chaotic part of phase space decreases again and is restricted to a thin layer separating and surrounding two regular islands, corresponding to two stable fixed points separated by an unstable one. Most orbits seem to lie on integrable tori. This suggests that the system has an integrable regime in the limit of small energies.

This limit corresponds to the hydrodynamical regime [14] investigated in several contexts. In a bulk case, when there is no external potential $U(x)$ the lowest lying excitations are phonons with linear wave-number dependence.

Numerically we have found that tending with the energy to zero, keeping $\mu$ fixed the range of the classical motion outside the condensate for trajectories starting inside is getting smaller and smaller and in the limit the motion is confined to the region inside of the Thomas-Fermi surface. Starting trajectories from the same point inside the condensate under the same direction and changing only the modulus of Cartesian-momentum we have found that they differ from each other only in a thin region near the boundary whose width scales with the energy. Lowering the modulus of the initial momentum to zero they tend to a well-defined limiting trajectory. This can be clearly seen in Fig. 2. In the isotropic case this is the limit $E/\mu, \omega_0 L/\mu \to 0$, keeping the ratio $L/E$ fixed. In the following section this 'hydrodynamic regime' will be studied in detail for anisotropic traps. However, it will turn out that in traps there exists a second low-energy regime, which for isotropic traps is defined by $E/\mu \to 0$ with $E - (\omega_0 L)^2/4\mu \ll E$, where the quasi-particles are single-particle like excitations confined to a narrow layer around the surface of the condensate. This low-energy Hartree-Fock regime will be discussed in detail in section IV, also for anisotropic traps, together with the usual high-energy ($E \gg \mu$) Hartree-Fock regime.

III. QUASI-PARTICLE DYNAMICS IN THE HYDRODYNAMIC REGIME

A. Hydrodynamic Hamiltonian

If there exist limiting trajectories for different initial conditions there should exist limiting dynamics described by some limiting Hamilton-function. Inside the condensate the Bogoliubov Hamiltonian can be written as

$$H(p, x) = \sqrt{\epsilon_{\text{kin}}(p)(\epsilon_{\text{kin}}(p) + 2K(x))},$$

(27)

where $\epsilon_{\text{kin}}(p) = p^2/2m$. For small energies $K(x)$ is much bigger than $\epsilon_{\text{kin}}$ everywhere except in a small region near the boundary. This suggests that the approximant of the Hamilton function (27) can be obtained by neglecting the kinetic energy square

$$H_{\text{hyd}}(p, x) = \sqrt{2 \epsilon_{\text{kin}}(p) K(x)}$$

(28)

for describing the motion in the hydrodynamical regime. This approximate Hamiltonian is in accordance with the bulk case, when $K(x) = \mu$ should be taken in (28) in order to obtain the linear phonon spectra from the Bogoliubov dispersion relation.

This Hamiltonian is meaningful only inside the condensate and only near the boundary of the condensate the full Hamiltonian (27) differs from this approximate one. On the Thomas-Fermi surface the full Hamilton function gives definite values for the Cartesian momenta, whereas according to $H_{\text{hyd}}$ they become infinite. Following the trajectories of $H_{\text{hyd}}$ in the isotropic case the angular momentum conservation requires that the tangential component of the momentum remains finite even though the absolute value of the momentum diverges like $K^{-1/2}$. Therefore each trajectory hits the boundary orthogonally and is reflected back orthogonally without change in the tangential component of the momentum. As this local rule is independent of the global symmetry of the trap potential it must hold also in the anisotropic case.

The Hamiltonian (28) has some further unusual features. The first observation is that it is not of the usual form but is a homogeneous first order function of the momenta. The strong consequence is that with the same initial value $x(t = 0)$ and with the same direction of the initial momenta the orbit $x(t)$ is the same independently of the energy. Secondly, a constraint follows from the canonical equations of motion, namely
\[ m\ddot{x} \cdot \dot{x} = \mu - U(x), \]  

relating the velocities and the coordinates. Thus one cannot choose the initial point and the velocity independently. Furthermore, due to this constraint one cannot express the three velocities in terms of the momenta, i.e., one cannot do the inverse Legendre transformation in the usual way to derive the Lagrangian. From (28) it is clearly seen that despite of the divergence of momenta on the boundary of the condensate the velocities even tend to zero here.

**B. Isotropic case**

In the isotropic trap case \((\omega_0 = \omega_x = \omega_y = \omega_z)\) the Poisson-bracket of \(H_{\text{hyd}}(p, x)\) (See Eq.(28)) and the angular momentum vector \(L\) is zero, which means that any components of \(L\) is a conserved quantity. Let us choose our coordinate system in such a way that the \(z\) axis is parallel with \(L\). In such a frame \(L_x = L_y = 0\), which shows that the motion in the phase space stays on the hypersurface \(z = p_z = 0\). By this choice of the coordinates one can eliminate one degrees of freedom from the Hamiltonian (28), which has then the form

\[ H_{\text{hyd}}(p, x) = \sqrt{\frac{\mu}{m} (p_x^2 + p_y^2)} (1 - \frac{x^2 + y^2}{r_{TF}^2}), \]  

where \(r_{TF}\) denotes the radial size of the condensate, the Thomas Fermi radius \(r_{TF} = \sqrt{\frac{2\mu}{m\omega_0^2}}\). Let us now consider the transformation

\[
\begin{align*}
x &= \frac{r_{TF}}{(I_1 + I_2)} (I_1 \cos \phi_1 + I_2 \cos \phi_2), \\
y &= \frac{r_{TF}}{(I_1 + I_2)} (I_1 \sin \phi_1 - I_2 \sin \phi_2), \\
p_x &= -\frac{r_{TF}}{I_1 + I_2} (I_1 + I_2) (\sin \phi_1 + \sin \phi_2), \\
p_y &= \frac{r_{TF}}{I_1 + I_2} (I_1 + I_2) (\cos \phi_1 - \cos \phi_2),
\end{align*}
\]

with positive \(I_1\) and \(I_2\). It is straightforward to check that the Poisson-brackets between \(I_1, I_2, \phi_1, \phi_2\) are canonical, thus, the transformation (31) is a canonical transformation. Inserting (31) into (30) one gets

\[ E = \frac{\mu}{2m} \sqrt{\frac{I_2}{I_1}} = \omega_0 \sqrt{2I_1 I_2}, \]  

i.e., \(I_1\) and \(I_2\) are the action and \(\phi_1\) and \(\phi_2\) the angle coordinates of the Hamiltonian (30). Similarly to the harmonic oscillator case this Hamiltonian is a homogeneous first order function of the action coordinates.

The Hamilton equations in the new coordinates are

\[
\begin{align*}
\dot{I}_1 &= 0, \\
\dot{\phi}_1 &= \frac{\omega_0}{\sqrt{2}} \sqrt{\frac{I_2}{I_1}} = \Omega_1, \\
\dot{I}_2 &= 0, \\
\dot{\phi}_2 &= \frac{\omega_0}{\sqrt{2}} \sqrt{\frac{I_1}{I_2}} = \Omega_2.
\end{align*}
\]

Using the above transformation, it is easy to show that the angular momentum is

\[ L_z = xp_y - yp_x = I_1 - I_2. \]  

A nice geometrical meaning for \(x(t)\) can be given. Let us consider a circle of radius \(b\), in which a smaller circle of radius \(a\) rolls. The motion of a point on the perimeter of the smaller circle in cartesian coordinates is described by the equations

\[
\begin{align*}
x &= (b - a) \cos \phi_1 + a \cos \phi_2, \\
y &= (b - a) \sin \phi_1 - a \sin \phi_2,
\end{align*}
\]  

where \(\phi_1\) and \(\phi_2\) are linear functions of the time, see Fig.3. Due to the perfect rolling condition the angular velocities are not independent.
Comparing the parametric form of the hypocycloid \([35]\) with \([31]\) it is obvious that \(x(t)\) fulfills \([35]\) and the constraint \([36]\), if \(b = r_{TF}, a = r_{TF}I_2/(I_1 + I_2)\), and if \(\phi_1, \phi_2\) are chosen as in \([33]\).

The radial distance from the origin can be expressed by

\[
r = \sqrt{x^2 + y^2} = \frac{r_{TF}}{I_1 + I_2} \sqrt{I_1^2 + I_2^2 + 2I_1I_2 \cos(\phi_1 + \phi_2)}.
\]

It is obvious that it is periodic in \((\phi_1 + \phi_2)\), its period can be calculated from

\[
T_r = \frac{2\pi}{\frac{E}{\hbar \sqrt{2E^2 + (L_z\omega_0)^2}}}.
\]

The Hamiltonian \([31]\) can be written in polar coordinates \(r, \phi\) as well. \(\phi\) is a cyclic variable, its conjugate momentum \(I_\phi = |L_z|\) is a conserved quantity. However, the momentum \(p_r = (xp_x + yp_y)/r\) conjugated to \(r\) is not conserved. To express the Hamiltonian \([31]\) in the action variables \(I_r, I_\phi\) let us use the fact that \(2\pi I_r = \oint p_r \, dr\) and that during one period of the radial motion \(\phi_1 + \phi_2\) changes by \(2\pi\). Using the above formulas one gets

\[
I_r = \min(I_1, I_2),
I_\phi = |I_1 - I_2|,
\]

which leads by \([32]\) to

\[
E = H_{hyd}(I_r, I_\phi) = \omega_0 \sqrt{2(I_r + I_\phi)} I_r.
\]

If one quantizes semiclassically the Hamiltonian \([40]\) one should take into account that in the radial direction there are two turning points, thus, \(I_r\) should be replaced by \(\hbar(n+1/2)\), and by the usual procedure for spherically symmetric problems \(I_\phi\) by \(\hbar(l + 1/2)\) \((l\) and \(n\) are non-negative integers). The semiclassical quantization leads by the above replacement rules to

\[
E_{n,l} = \hbar \omega_0 \sqrt{2n^2 + 2nl + 3n + l + 1},
\]

which is almost that of the result of Stringari \([10]\), except the 1 under the square-root, and agrees with that of the more elaborate semiclassical quantization in the hydrodynamical limit \([3]\).

**C. Anisotropic case with cylindrical symmetry**

The case of a trap with axial or cylindrical symmetry is the experimentally most relevant one. In Poincaré cuts of the full dynamics we have seen regular behaviour for small energies. Therefore one can expect that the classical motion given by the approximate Hamiltonian is fully integrable. To show this let us introduce new coordinates, namely the cylindrical elliptical coordinates \(\xi, \eta\) given by

\[
\rho = \sigma \sqrt{(\xi^2 + 1)(1 - \eta^2)} \quad , \quad z = \sigma \xi \eta
\]

which are orthogonal coordinates. Surfaces of constant \(\xi\) are confocal ellipsoids with foci at a distance \(\sigma\) in \(\rho\) direction, surfaces of constant \(\eta\) are confocal hyperboloids with the same foci. For \(\sigma\), the parameter of the transformation, we take the foci of the Thomas-Fermi ellipsoid, \(\sigma = \epsilon(2\mu/m\omega_0^2)^{1/2}\) for \(\omega_z > \omega_0\). For \(\omega_0 > \omega_z\) one has to change \(\xi^2 + 1\) to \(\xi^2 - 1\) and take \(\sigma = \epsilon(2\mu/m\omega_z^2)^{1/2}\). In the following we consider only the first case \([12]\), in the second case the analysis proceeds similarly. \(\xi\) can take any value in the range \([0, (1/\epsilon^2 - 1)^{1/2}]\). The limiting case \(\xi = (1/\epsilon^2 - 1)^{1/2}\) describes the Thomas-Fermi ellipsoid. \(\eta\) can be in the range \([-1, 1]\). Making the point transformation from cylindrical to cylindrical elliptical coordinates the momenta transform as

\[
p_\rho = \frac{1}{\sigma \xi^2 + \eta^2} \sqrt{(\xi^2 + 1)(1 - \eta^2)} (\xi p_\xi - \eta p_\eta), \quad p_z = \frac{1}{\sigma \xi^2 + \eta^2} ((\xi^2 + 1)\eta p_\xi + (1 - \eta^2)\xi p_\eta).
\]
The Hamiltonian \((28)\) in cylindrical elliptical coordinates is
\[
H_{hyd} = \frac{\omega^2}{2\epsilon^2} \left( 1 - \epsilon^2(\xi^2 + 1) \right) \frac{1}{\xi^2 + \eta^2} \left( (\xi^2 + 1)\dot{\xi}^2 + (1 - \eta^2)\dot{\eta}^2 + \frac{1}{\xi^2 + 1}\dot{p}_\phi^2 \right).
\]

Taking the energy \(E\) and \(p_\phi = L_\phi\) as constants one can write down the Hamilton-Jacobi equation for \(\xi\) and \(\eta\), which is separable in these coordinates. Thus the problem is fully integrable. Introducing a separation constant \(B > 0\) the two separated Hamilton-Jacobi equations are
\[
(\xi^2 + 1) \left( \frac{dS}{d\xi} \right)^2 - \frac{L_\xi^2}{\xi^2 + 1} - \frac{2E^2}{\omega^2} \frac{1}{1 - \epsilon^2(\xi^2 + 1)} = -B
\]
\[
(1 - \eta^2) \left( \frac{dS}{d\eta} \right)^2 + \frac{L_\eta^2}{1 - \eta^2} + \frac{2E^2}{\omega^2} \frac{1}{1 - \epsilon^2(1 - \eta^2)} = B.
\]

Combining these two equations one gets for the separation constant \(B\) the phase-space function
\[
B = \frac{1}{\epsilon^2} \frac{1}{\xi^2 + \eta^2} \left[ (1 - \epsilon^2(\xi^2 + 1))(\xi^2 + 1)p_\xi^2 + (1 - \epsilon^2(1 - \eta^2))(1 - \eta^2)p_\eta^2 + \left( \frac{1}{\xi^2 + 1} - \frac{1}{\xi^2 + 1}\right)p_\phi^2 \right]
\]
\[
= \frac{\sigma^2}{\epsilon^2} \left[ p_\xi^2 + p_\eta^2 + (1 - \epsilon^2)p_\phi^2 \right] - (xp_x + yp_y + zp_z)^2.
\]

in elliptical and cartesian coordinates respectively. This is the third independent constant of motion in addition to the energy \(E\) and \(L_\phi\). This can be checked directly, using the equations of motion for the time derivatives of \(x, y, z\) and therefore the almost integrable situation found numerically in the motion generated by the total Hamiltonian \((27)\) in the small energy and small angular momentum region. We notice that two kinds of trajectories can occur in this regime. From \((45)\) we can determine the turning points in \(\xi\) and \(\eta\). In \(\xi\)-direction all the trajectories reach the Thomas-Fermi surface and are reflected back there. If the condition
\[
B > B^* = \frac{2E^2}{\omega_0^2} + L_\phi^2,
\]
is satisfied, there is an inner turning point in \(\xi\)-direction and \(\eta\) takes a range \([-\eta_{max}, \eta_{max}]\). These trajectories correspond to the hypocycloids of the isotropic case, as an example see Fig.4a. For \(B < B^*\) however there are further turning points in \(\eta\)-direction, the motion being confined between two hyperbolas with \(\xi\) values extending to zero, which can be seen in Fig.4b. This kind of trajectory only occurs in the anisotropic system. \(B = B^*\) is the separatrix between these two types of motion. As usual this separatrix is structurally unstable against small nonintegrable perturbations of the integrable motion in the hydrodynamic limit. It plays a crucial role for the appearance of chaos in the Bogoliubov Hamiltonian as the energy is increased from values very small compared to \(\mu\), because it is destroyed and replaced by a chaotic separatrix layer, which is very narrow at first, but grows in width as the energy is increased. In Fig.4c two regular islands corresponding to the two kinds of trajectories and the chaotic separatrix layer between them can be seen.
D. Completely anisotropic case

The analysis of the preceding section can be generalized to the case of a completely anisotropic harmonic trap. The formulas become rather lengthy and we just indicate the essential steps.

The trap potential is written in the form

$$U(x) = \mu \left( \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} \right)$$  \hspace{1cm} (49)

with

$$a^2 = 2\mu/m\omega_x^2 \hspace{1cm} \text{ (and cyclic).} \hspace{1cm} (50)$$

We may assume \(a > b > c\) without restriction of generality. Then new elliptic coordinates \(\xi, \eta, \zeta\) are introduced via

$$x = \pm \sqrt{\frac{(a^2 + \xi)(a^2 + \eta)(a^2 + \zeta)}{(a^2 - b^2)(a^2 - c^2)}} \hspace{1cm} \text{ (and cyclic)} \hspace{1cm} (51)$$

after which the potential reads

$$U(\xi, \eta, \zeta) = \mu(1 + \frac{\xi\eta\zeta}{a^2b^2c^2}).$$ \hspace{1cm} (52)

The range of \(\xi, \eta, \zeta\) is \(0 \leq \xi \geq -c^2 \geq \eta \geq -b^2 \geq \xi \geq -a^2\). The old canonical momenta \(p_x, p_y, p_z\) are given in terms of the new ones by

$$p_x = \sqrt{\frac{(a^2 + \xi)(a^2 + \eta)(a^2 + \zeta)}{(a^2 - b^2)(a^2 - c^2)}} \left[ 2p_\xi \frac{(b^2 + \xi)(c^2 + \xi)}{(\xi - \eta)(\xi - \zeta)} \right] \hspace{1cm} \text{ (and cyclic)} \hspace{1cm} (53)$$

Then the Hamiltonian in the hydrodynamic limit can be written in terms of the new canonical coordinates and momenta. The Hamilton-Jacobi equation can be written in the nearly separated form

$$0 = (\eta - \zeta) \left[ (a^2 + \xi)(b^2 + \xi)(c^2 + \xi) \frac{\partial S}{\partial \xi} + \frac{E^2m}{4\mu} \frac{a^2b^2c^2}{\xi} \right] + \text{ (cyclic).} \hspace{1cm} (54)$$

In fact complete separation is achieved, because this equation is satisfied only by putting the angular brackets equal to \(A + B\xi\) (and cyclic),

$$\left[ (a^2 + \xi)(b^2 + \xi)(c^2 + \xi)p_x^2 + \frac{E^2m}{4\mu} \frac{a^2b^2c^2}{\xi} \right] = \frac{1}{4} (A + B\xi) \hspace{1cm} \text{ (and cyclic)} \hspace{1cm} (55)$$

where \(A\) and \(B\) are two separation constants, which are the same for all three equations related by cyclic permutation. From these three equations \(A\) and \(B\) can be eliminated by multiplying the first with \((\eta - \zeta)\), the second with \((\zeta - \xi)\), the third with \((\xi - \eta)\) and adding them. This gives, of course, back eq. (54), which defines \(E = H_{\text{hyd}}\) in terms of the canonical variables. However, solving the three equations instead for \(A\) by eliminating \(B\) and \(E\), and then for \(B\) eliminating \(A\) and \(E\) we obtain two new conserved phase-space functions. Translated back to Cartesian coordinates these read

$$A = -\{[(b^2 + c^2)(x^2 - a^2) + a^2(y^2 + z^2)]p_x^2 + 2a^2 yz p_y p_z \} + \text{ (cyclic)} \hspace{1cm} (56)$$

and

$$B = -\{(x^2 - a^2)p_x^2 + 2yz p_y p_z \} + \text{ (cyclic)}. \hspace{1cm} (57)$$

The conserved function \(B\) is a simple generalization of the conservation law we already found in the case with cylindrical symmetry, whereas \(A\) corresponds to \(L_z^2\). By a straightforward but lengthy calculation it can be checked that the Poisson brackets \(\{H_{\text{hyd}}, A\}, \{H_{\text{hyd}}, B\}, \{A, B\}\) all vanish. Therefore, the dynamics governed by \(H_{\text{hyd}}\) is still completely integrable even in this completely anisotropic case.
IV. THE HARTREE-FOCK DYNAMICS

Another limiting case of the Bogoliubov description of quasiparticles [1] consists in neglecting the hole-component $V_j(x)$ in the field operator $\hat{\varphi}(x)$. The remaining component $U_j(x)$ is then described by the Hartree-Fock Hamiltonian [1]. The interaction between particles is taken into account by the potential $K(x)$, describing the mean interaction of one particle with all the other particles. Restricting ourselves to $T = 0$ all those other particles are in the condensate. In the homogenous systems this approach simply results in a shift of the dispersion relation of noninteracting particles by the chemical potential $\mu$. For spatially homogeneous Bose condensates and also Bose condensates in traps such a description can be applied for energies larger than the mean interaction energy given by $\mu$. However, in traps there is even a regime for energies smaller than $\mu$ where the Hartree-Fock approximation applies [1], namely in the case when the kinetic energy $\epsilon_{kin}(p)$ is large compared to the local mean interaction energy $K(x)$. This can be satisfied in a layer around the surface of the Bose condensate where $K(x)$ is very small.

Using the Thomas-Fermi approximation for the wave function $\tilde{\psi}$ the Bogoliubov Hamiltonian and the Hartree-Fock Hamiltonian coincide outside the condensate. Inside the condensate, if the kinetic energy $\epsilon_{kin}(p)$ is much larger than the potential term $K(x)$, an expansion of the Bogoliubov Hamiltonian $H_{BF}$ to first order in $K(x)$ just gives the Hartree-Fock Hamiltonian

$$H_{HF} = \frac{p^2}{2m} + |U(x) - \mu|,$$

which is therefore valid, for $\epsilon_{kin} \gg K(x)$, inside and outside the condensate.

We now want to investigate the classical dynamics of this Hartree-Fock Hamiltonian. The isotropic problem is completely integrable again. As constants of motion we can take the energy, the modulus and the conjugate momentum $p_\eta$ and its elliptical coordinate $\eta$. For energies much larger than the chemical potential the interaction with the condensate is only a small perturbation to the integrable motion in the harmonic trap and we observe quasi-regular behaviour. In this limit the Bogoliubov description of quasi-particles reduces to the Hartree-Fock description, the condensate is only a small perturbation to the integrable motion in the harmonic trap and we observe quasi-regular behaviour. From this we can conclude that the stochasticity observed for the Bogoliubov Hamiltonian in Fig.3 [2] is not a consequence of the coupled two component structure of the underlying semiclassical description, but is simply caused by the anisotropy of the external potential.

For energies much smaller than the chemical potential $E < 0.1\mu$ we find regular behaviour again, see Fig.5b. Particles are confined to the sharp potential channel near the Thomas-Fermi surface. The width of this potential channel scales as $E/\mu$. Roughly the particles spend the same time outside and inside the condensate. We look at the problem in elliptical coordinates (42), and choose for concreteness again the case $\omega_z > \omega_\eta$. The oscillations in $\xi$ orthogonal to the Thomas-Fermi surface $\xi = (1/c^2 - 1)^{1/2}$ are much faster than the oscillations in $\eta$-direction along the channel. This suggests to make an adiabatic approximation in which the action-integral $I_\xi = (2\pi)^{-1} \oint p_\xi d\xi$ over one full cycle in $\xi$ at fixed $\eta$, $p_\eta$ emerges as an adiabatic constant for the motion. Evaluating this adiabatic invariant for $E/\mu \ll 1$ we get as a function of $\eta$, $p_\eta$

$$I_\xi = \frac{4\mu}{3\pi \omega_z} \frac{1}{\sqrt{1 - c^2(1 - \eta^2)}} \left( \frac{E}{\mu} - \frac{1 - \eta^2}{1 - c^2(1 - \eta^2)} \frac{(\omega_\eta p_\eta)^2}{2\mu} - \frac{1}{1 - \eta^2} \frac{(\omega_\eta L_z)^2}{2\mu} \right)^{3/2}.$$

This new adiabatically conserved quantity which emerges in the low-energy limit of the Hartree-Fock dynamics, is the cause of integrability in that limit.

Solving this equation for the energy we get the Hamiltonian of the slow $\eta$-dynamics, valid for low energies. From (25) we see that the turning points in $\eta$ are independent of the energy if we keep $L_z/E^2$ and $I_\xi/E^{3/2}$ constant. In Fig.5b we compare a Poincaré section in $\eta$ and $p_\eta$ of the dynamics of the Hartree-Fock Hamiltonian with trajectories of the slow $\eta$-dynamics for different values of $I_\xi$. Both curves agree very well. For smaller energies $E \leq 0.01\mu$ no difference between both curves can be noticed.

Now we have to ask ourselves, which of the trajectories displayed in Fig.5b are indeed good approximations to trajectories described by the Bogoliubov Hamiltonian. Let us look first at the isotropic case, where the motion
separates in radial and angular motion. The kinetic energy in the angular degree of freedom roughly is \( L^2/2m r^2 \approx (\omega_0 L)^2/4\mu \). Since for low energies \( r \) deviates only very little from the Thomas-Fermi radius this rotational energy is almost conserved. The remaining energy is stored in the radial degree of freedom and only this energy can be transformed to potential energy. So the condition that the Hartree-Fock dynamics and the Bogoliubov dynamics agree is in this case

\[
E - \frac{(\omega_0 L)^2}{4\mu} \ll E .
\]

For the anisotropic case we can formulate an analogous criterion: Only if most of the energy is kinetic energy of the motion parallel to the boundary, which cannot be transformed into potential energy, the approximation of the Bogoliubov dynamics by the Hartree-Fock dynamics works well. For \( I_\xi = 0 \) no motion takes place orthogonal to the surface, \( \xi \) being constant, and all the energy is stored in motion parallel to the surface. This corresponds to the outer orbit forming the boundary of the cut in Fig.5. The maximal value of \( I_\xi \) for fixed \( L_z \) is given by setting \( \eta = p_\eta = 0 \) in (60). This trajectory corresponds to the origin of Fig.5, where motion takes only in \( \xi \) and \( \phi \) directions. Generally the two dynamics differ in this case, unless most of the energy is stored in angular motion of the cyclic variable \( \phi \) which is also motion along the Thomas-Fermi surface. The maximal value of \( I_\xi \) for a given energy is found by neglecting both angular motions in \( \eta \) and in \( \phi \) in (60), by putting \( p_\eta, L_z \) equal to zero there. As a condition that only a small fraction of energy is stored in the motion orthogonal to the surface and hence that both motions from the Bogoliubov and from the Hartree-Fock Hamiltonian agree, we can thus state:

\[
I_\xi \ll I_\xi^{\text{max}} = \frac{4\mu}{3\pi \omega_0} \left( \frac{E}{\mu} \right)^{3/2} .
\]

In Fig.5 we compare Poincaré cuts of the Bogoliubov dynamics with the one-degree of freedom motion obtained from (61), representing the integrable Hartree-Fock dynamics for small energies. We see that indeed both dynamics agree well for small values of \( I_\xi \) near the boundary of the cut. For \( L_z \) chosen large, see Fig.5a, even for values of \( I_\xi \) close to the maximal one, both dynamics in \( \eta \) agree qualitatively. However the different behaviour in the variable \( \xi \) orthogonal to the surface can, of course, not be seen in this cut at constant \( \xi \). For smaller values of \( L_z \), see Fig.5b, we can distinguish two regions. Near the boundary, for small \( I_\xi \), we see the Hartree-Fock limit of the Bogoliubov dynamics, where both dynamics agree. The inner region corresponds to the hydrodynamic limit of the Bogoliubov dynamics and cannot be compared with the Hartree-Fock dynamics. The two kinds of closed tori visible here are the two kinds of hydrodynamic trajectories discussed at the end of section III.C.

V. CONCLUSIONS

The quasi-particle excitations are the basic constituents of the dynamical and thermodynamical properties of Bose condensates. In the present paper we have investigated their dynamics for Bose condensates of atomic gases in traps in the classical limit. The two limiting types of excitations, collective modes and quasi-particle excitations consisting essentially of single atoms moving in a mean field correspond, in the classical limit, to particles and anti-particles of zero mass, moving ‘relativistically’ with the speed of sound, and to single atoms moving in the potential created by the trap and the Hartree-Fock potential energy of all other atoms. In spatially homogeneous (untrapped) condensates these two types of excitation strongly differ in energy \( E \), the collective modes occurring at \( E \ll \mu \), the single-particle modes at \( E \gg \mu \). In the trapped condensates both types of excitations coexist, at least classically, at small energies \( E \ll \mu \), and are instead spatially separated. The collective modes live inside the condensate, the single-particle modes at small energies in a narrow layer at the border.

One principal result we have obtained here is that the classical dynamics of both, the collective modes and the single-particle modes, become integrable in the limit \( E/\mu \ll 1 \). This has important consequences for the quantum dynamics as well: the integrability can be used there to separate the Schrödinger equation and to obtain not only the low-lying levels of the collective modes \( 11 \), but also of the single-particle modes. After quantization an energy gap reappears separating the collective modes with typical energies \( \hbar \omega_0 \) and the single-particle modes whose lowest levels have energies of the order \( (\hbar \omega_0)^{2/3} \mu^{1/3} \) due to their close confinement in normal direction to the surface of the condensate. However, this energy difference is much smaller than, and has a different origin as the energy difference between both types of modes in homogeneous systems.

Another principal result obtained here is the nonintegrability of the classical dynamics of the quasi-particle excitations at intermediate energies \( E \simeq \mu \). This applies to both, the full Bogoliubov dynamics and the limiting Hartree-Fock dynamics approximating it wherever the kinetic energy is large compared to the local mean interaction energy. Again
this nonintegrability has a direct consequence also for the quantum dynamics, because it implies avoided crossings between quasi-particle levels as functions of the dimensionless interaction strength $N_0a/d_0$ with $d_0 = \sqrt{\hbar/m\omega_0}$, if the energy and $\mu$ are comparable. Such avoided crossings have indeed been seen in numerically generated plots [14].

Our results not only explain these avoided crossings, they also open the door to an intriguing wider perspective, quantum chaos of the quasi-particle dynamics in the Bose condensates of atoms in anisotropic traps.

ACKNOWLEDGEMENTS

This work has been supported by the project of the Hungarian Academy of Sciences (grant No. 95) and the Deutsche Forschungsgemeinschaft. M.F. gratefully acknowledges support by the German-Hungarian Scientific and Technological Cooperation under Project 62. R.G. and M. F. wishes to acknowledge support by the Deutsche Forschungsgemeinschaft through the Sonderforschungsbereich 237 “Unordnung und große Fluktuationen”. Two of us (A.Cs.,P.Sz.) would like to acknowledge support by the Hungarian Academy of Sciences under grant No. AKP 96-12/12. The work has been partially supported by the Hungarian National Scientific Research Foundation under grant Nos. OTKA T017493, F020094 and by the Ministry of Education of Hungary under grant No. FKFP0159/1997.

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FIG. 1. Poincaré sections of the dynamics of the Bogoliubov Hamiltonian (21) in cylindrical coordinates for the different energies (from top to bottom) $E/\mu = 40$ (a), 1 (b) and 0.02 (c). The cut is taken at $z = 0$ and displayed in the variables $p_\rho$, $p_{\rho}^{1/2}$, $(2\mu)^{1/2}$, respectively. The anisotropy is chosen as $\omega_z/\omega_0 = \sqrt{5}$, the angular momentum was fixed as $0.2L_z/E = 0.2$.

FIG. 2. Trajectories in coordinate space of the Bogoliubov dynamics of (21) starting from the same point and in the same direction for different energies $E/\mu = 0.1$ (dashed line), 0.01 (solid) and $10^{-4}$ (dotted).

FIG. 3. Coordinates for the hypocycloid (35).
FIG. 4. Trajectory of the hydrodynamic Hamiltonian (28) for $B > B^*$ (a) and for $B < B^*$ (b). $z, \rho$ are plotted in units of $(2\mu/m\omega_0^2)^{1/2}$.

FIG. 5. Poincaré section of the dynamics of the Hartree-Fock Hamiltonian (58) in elliptical coordinates (42) for the energy $E/\mu = 1$ (a) and $E/\mu = .06$ (b). The cut is taken on the Thomas-Fermi surface in the variables $\eta, p_\eta$ for $\omega_z/\omega_0 = \sqrt{3}$. The angular momentum is given by $(\omega_0 L_z)^2/2\mu E = 1$. Solid lines in (b) are trajectories of the Hamiltonian in $(\eta, p_\eta)$ following from (59).

FIG. 6. Poincaré sections of the dynamics of the Bogoliubov Hamiltonian (21) in elliptical coordinates (42) for the energies $E/\mu = 0.1$ with $(\omega_0 L_z)^2/2\mu E = 1$ (a) and $E/\mu = 0.01$ with $(\omega_0 L_z)^2/2\mu E = 0.02$ (b) on the Thomas-Fermi surface in $\eta, p_\eta$ for $\omega_z/\omega_0 = \sqrt{3}$. Solid lines are trajectories of the Hamiltonian in $(\eta, p_\eta)$ following from (59).
