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Low-energy elementary excitations of a trapped Bose-condensed gas

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We develop a method of finding analytical solutions of the Bogolyubov-de Gennes equations for the excitations of a Bose condensate in the Thomas-Fermi regime in harmonic traps of any asymmetry and introduce a classification of eigenstates. In the case of cylindrical symmetry we emphasize the presence of an accidental degeneracy in the excitation spectrum at certain values of the projection of orbital angular momentum on the symmetry axis and discuss possible consequences of the degeneracy in the context of new signatures of Bose-Einstein condensation. [S1050-2947(97)51410-7]

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The recent realization of Bose-Einstein condensation (BEC) in trapped alkali-metal atom gases [1-3], followed by the second generation of experiments [4-8], has opened the possibility of investigating macroscopic quantum phenomena in these systems. For understanding the macroscopic quantum behavior of a trapped Bose-condensed gas, especially important is the character of elementary excitations of the trapped condensate, which to a large extent is predetermined by the interaction between atoms. In dilute gases the interaction is primarily binary and is characterized by a single parameter a, the s-wave scattering length. This allows one to develop a transparent theory that can be tested experimentally.

At present theoretical investigations of elementary excitations of trapped Bose condensates include analytical solutions for the spectrum of low-energy excitations in spherically symmetric harmonic traps in the Thomas-Fermi regime [9] and numerical analysis of the eigenfunctions and eigenenergies of the excitations in the traps of spherical and cylindrical symmetry [10-14]. In the latter case the eigenfrequencies of the lowest excitations, as those measured by Jin *et al.* [4,8] and Mewes *et al.* [7] in experiments, they have also been found analytically [9,15,16,13].

Most interesting are the low-energy excitations, i.e., the excitations with energies much smaller than the chemical potential (mean-field interaction between particles), as they are essentially of collective character. Previous studies revealed that the eigenfrequencies of condensate oscillations are strongly different from those of a collisionless thermal gas [4,7,8], but are rather close to the frequencies of a thermal gas in the hydrodynamic regime [16,17]. In this paper we develop a method of finding analytical solutions of the Bogolyubov-de Gennes equations for the spectrum and wave functions of the condensate excitations in the Thomas-Fermi regime in harmonic traps of any type of asymmetry and introduce a classification of eigenstates. We analyze the structure of the excitation spectrum in the case of cylindrical symmetry and find an accidental degeneracy at certain values of the projection of orbital angular momentum on the symmetry axis. We address the question of how the accidental degeneracy can manifest itself, providing us with a clear distinction between the condensate oscillations and the oscillations of a classical gas in the hydrodynamic regime.

We consider a Bose-condensed gas in an external harmonic potential $V(\mathbf{r}) = M \sum_i \omega_i^2 r_i^2 / 2$ with frequencies ω_i and assume a pair potential of the atom-atom interaction of the form $U(\mathbf{R}) = \widetilde{U}\delta(\mathbf{R})$, where $\widetilde{U} = 4\pi\hbar^2 a/M$, a is the scattering length, and M the atom mass. Then the grand-canonical Hamiltonian of the system is written as

$$\hat{H} = \int d\mathbf{r} \,\hat{\Psi}^{\dagger}(\mathbf{r}) \bigg[-\frac{\hbar^2}{2M} \Delta + V(\mathbf{r}) - \mu + \frac{1}{2} \widetilde{U} \,\hat{\Psi}^{\dagger}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \bigg] \\ \times \hat{\Psi}(\mathbf{r}) \,, \tag{1}$$

where $\Psi(\mathbf{r})$ is the field operator of atoms, and μ the chemical potential. The field operator can be represented as a sum of the above-condensate part and the condensate wave function $\Psi_0 = \langle \Psi \rangle$, which is a *c* number: $\hat{\Psi} = \hat{\Psi}' + \Psi_0$ (see [18]). Assuming that the condensate density greatly exceeds the density of above-condensate particles we omit the terms proportional to $\hat{\Psi}^{\prime 3}$ and $\hat{\Psi}^{\prime 4}$ in Eq. (1) and write the Hamiltonian in the form

$$\hat{H} = \hat{H}_{0} + \int d\mathbf{r} \left\{ \hat{\Psi}'^{\dagger}(\mathbf{r}) \left[-\frac{\hbar^{2}}{2M} \Delta + V(\mathbf{r}) - \mu \right] \hat{\Psi}' + \frac{1}{2} \widetilde{U} [4|\Psi_{0}(\mathbf{r})|^{2} \hat{\Psi}'^{\dagger}(\mathbf{r}) \hat{\Psi}'(\mathbf{r}) + \Psi_{0}^{2} \hat{\Psi}'^{\dagger}(\mathbf{r}) \hat{\Psi}'^{\dagger}(\mathbf{r}) + \Psi_{0}^{*2} \hat{\Psi}'^{\dagger}(\mathbf{r}) \hat{\Psi}'^{\dagger}(\mathbf{r}) \right] \right\}, \qquad (2)$$

$$\hat{H}_{0} = \int d\mathbf{r} \Psi_{0}^{*}(\mathbf{r}) \left[-\frac{\hbar^{2}}{2M} \Delta + V(\mathbf{r}) - \mu + \frac{1}{2} \widetilde{U} |\Psi_{0}(\mathbf{r})|^{2} \right] \\ \times \Psi_{0}(\mathbf{r}) .$$
(3)

The Gross-Pitaevskii equation for Ψ_0 normalized by the condition $\int |\Psi_0(\mathbf{r})|^2 d\mathbf{r} = N_0 (N_0 \text{ is the number of particles in the})$ condensate) follows directly from \hat{H}_0 in Eq. (3),

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$$\left(-\frac{\hbar^2}{2M}\Delta + V(\mathbf{r}) + \widetilde{U} |\Psi_0|^2\right) \Psi_0 = \mu \Psi_0.$$
(4)

Owing to Eq. (4) the part of the Hamiltonian, which is linear in $\hat{\Psi}'$ [and not included in Eq. (2)], becomes equal to zero. The Hamiltonian (2) is bilinear in the operators $\hat{\Psi}'$, $\hat{\Psi}'^{\dagger}$ and can be reduced to a diagonal form

$$\hat{H} = H_0 + \sum_{\nu} E_{\nu} \hat{b}_{\nu}^{\dagger} \hat{b}_{\nu}$$
(5)

by using the Bogolyubov transformation generalized to an inhomogeneous case: $\hat{\Psi}'(\mathbf{r}) = \sum_{\nu} [(u_{\nu}(\mathbf{r})\hat{b}_{\nu} - v_{\nu}^{*}(\mathbf{r})\hat{b}_{\nu}^{\dagger}]$ [19]. Here \hat{b}_{ν} , \hat{b}_{ν}^{\dagger} are creation and annihilation operators of elementary excitations. The Hamiltonian takes the form (5) if the functions u_{ν} , v_{ν} satisfy the equations

$$\left(-\frac{\hbar^2}{2M}\Delta + V(\mathbf{r})\right)u_{\nu} + \widetilde{U}|\Psi_0|^2(2u_{\nu} - v_{\nu}) = (\mu + E_{\nu})u_{\nu}, \quad (6)$$

$$\left(-\frac{\hbar^2}{2M}\Delta + V(\mathbf{r})\right)v_{\nu} + \widetilde{U}|\Psi_0|^2(2v_{\nu} - u_{\nu}) = (\mu - E_{\nu})v_{\nu} \quad (7)$$

 $(\Psi_0 \text{ is taken real})$, and are normalized by the condition

$$\int d\mathbf{r}(u_{\nu}u_{\nu'}^{*} - v_{\nu}v_{\nu'}^{*}) = \delta_{\nu\nu'}.$$
 (8)

The Hamiltonian (5) does not contain the recently discussed term originating from the presence of the "momentum" operator of the condensate [20], since this term does not affect the elementary excitations.

Equations (6), (7), and (4) represent a complete set of equations for finding the wave functions u_v, v_v and energies E_v of the excitations. We will discuss the case of repulsive (a>0) interparticle interaction in the Thomas-Fermi regime $(\mu \approx n_{0m} \widetilde{U} \gg \hbar \omega_i, n_{0m}$ is the maximum condensate density), where the presence of a small parameter

$$\zeta = \hbar \,\overline{\omega} / 2\mu \ll 1 \tag{9}$$

 $(\overline{\omega} = \prod_i \omega_i^{1/3})$ allows us to simplify the equations for the elementary excitations. First, we write Eqs. (6), (7), and (4) in terms of dimensionless eigenenergies $\varepsilon_{\nu} = E_{\nu}/\hbar \overline{\omega}$ and coordinates $y_i = r_i/l_i$, where $l_i = (2 \mu/m \omega_i^2)^{1/2}$ is the characteristic size of the condensate in the *i*th direction:

$$-\zeta^{2}\widetilde{\Delta u}_{\nu} + y^{2}u_{\nu} + (2u_{\nu} - v_{\nu})\overline{n_{0}} = (1 + 2\zeta\varepsilon_{\nu})u_{\nu}, \quad (10)$$

$$-\zeta^2 \widetilde{\Delta} v_{\nu} + y^2 v_{\nu} + (2v_{\nu} - u_{\nu}) \overline{n_0} = (1 - 2\zeta \varepsilon_{\nu}) v_{\nu}, \quad (11)$$

$$-\zeta^{2}\widetilde{\Delta\Psi}_{0} + y^{2}\Psi_{0} + \overline{n_{0}}\Psi_{0} = \Psi_{0}.$$
 (12)

Here $\widetilde{\Delta} = \sum_i (\omega_i / \overline{\omega})^2 \partial^2 / \partial y_i^2$, and $y^2 = \sum_i y_i^2$. With the dimensionless condensate density $\overline{n_0} = |\Psi_0(\mathbf{r})|^2 / n_{0m}$ from Eq. (12), Eqs. (10) and (11) are reduced to the fourth-order differential equations for the functions $f_{\nu\pm} = u_{\nu} \pm v_{\nu}$:

$$(1-y^{2})\left\{-\widetilde{\Delta}f_{+}+f_{+}\frac{\widetilde{\Delta}\Psi_{0}}{\Psi_{0}}\right\}+\frac{\zeta^{2}}{2}\left[\widetilde{\Delta}^{2}f_{+}-3\frac{\widetilde{\Delta}\Psi_{0}}{\Psi_{0}}\widetilde{\Delta}f_{+}\right]$$
$$-\widetilde{\Delta}\left(f_{+}\frac{\widetilde{\Delta}\Psi_{0}}{\Psi_{0}}\right)+3\left(\frac{\widetilde{\Delta}\Psi_{0}}{\Psi_{0}}\right)^{2}f_{+}\right]=2\varepsilon^{2}f_{+},\qquad(13)$$

$$\begin{cases} -\widetilde{\Delta}(1-y^2)f_- + (1-y^2)f_- \frac{\Delta \Psi_0}{\Psi_0} \right\} + \frac{\varsigma}{2} \left[\widetilde{\Delta}^2 f_- - \frac{\widetilde{\Delta}\Psi_0}{\Psi_0} \widetilde{\Delta}f_- - 3\widetilde{\Delta} \left(f_- \frac{\widetilde{\Delta}\Psi_0}{\Psi_0} \right) + 3 \left(\frac{\widetilde{\Delta}\Psi_0}{\Psi_0} \right)^2 f_- \right] \\ = 2\varepsilon^2 f_- \,. \tag{14}$$

Here we have omitted the index ν and written the terms proportional to ζ^2 separately.

The low-energy excitations ($E \ll \mu$ or $\varepsilon \zeta \ll 1$) are primarily localized inside the condensate spatial region. At characteristic distances from the condensate boundary

$$\delta y \gg \max[\varepsilon \zeta, (\zeta/\varepsilon)^{1/2}],$$
 (15)

we can omit all terms proportional to ζ^2 in Eqs. (13) and (14), and use the Thomas-Fermi approximation for the condensate wave function (see [21,22])

$$\Psi_0 = \sqrt{n_{0m}(1 - y^2)}, \quad y \le 1, \tag{16}$$

following from Eq. (4) in which the kinetic energy term $\zeta^2 \tilde{\Delta} \Psi_0$ is neglected. Then, using the substitution $f_{\pm}(y) = C_{\pm}(1-y^2)^{\pm 1/2} W(y)$, we obtain the equation

$$\hat{G}W + 2\varepsilon^2 W = 0, \qquad (17)$$

where the operator \hat{G} is given by

$$\hat{G} = (1 - y^2) \widetilde{\Delta} - 2 \sum_i y_i (\omega_i / \overline{\omega})^2 \partial \partial y_i.$$
(18)

The relation between the normalization coefficients C_+ and C_- follows from Eqs. (10), (11), (17), and (18):

$$C_{-} = \varepsilon \zeta C_{+} \,. \tag{19}$$

The solution (16) can be used in Eqs. (10) and (11) from the very beginning for finding the wave functions and spectrum of elementary excitations with energies $E_v \gg \hbar \omega_i$. However, for the excitations with energies comparable to the trap frequencies, this would lead to an incorrect result. The reason is that the wave functions of such excitations vary over a distance comparable with the size of the condensate. Hence, the kinetic energy of the condensate, omitted in the derivation of Eq. (16), and the kinetic energy of the excitations are equally important. This is taken into account in our derivation of Eqs. (13) and (14), relying on the exact expression for Ψ_0 . In principle, the exact equations (13) and (14) can be used to obtain a systematic expansion of the excitation wave functions and energies in the ζ parameter.

In the case of spherical symmetry $(\omega_i = \overline{\omega} = \omega)$ the excitations are characterized by the orbital angular momentum land its projection m. The solution of Eq. (17) has the form R3348

$$x(1-x)\frac{d^2P}{dx^2} + \left[l + \frac{3}{2} - \left(l + \frac{5}{2}\right)x\right]\frac{dP}{dx} + \left(\frac{\varepsilon^2}{2} - \frac{l}{2}\right)P = 0.$$
(20)

The solution of Eq. (20), convergent at x=0, is the hypergeometric function that converges at $x \rightarrow 1$ only when reduced to a polynomial. This immediately gives the energy spectrum

$$E_{nl} = \hbar \,\omega \varepsilon_{nl} = \hbar \,\omega (2n^2 + 2nl + 3n + l)^{1/2}, \qquad (21)$$

where *n* is a positive integer. The solutions of Eq. (20) are classical Jacobi polynomials $P_n^{(l+1/2,0)}(1-2y^2)$ and, with the normalization conditions (8) and (19), we obtain

$$f_{\pm} = \left[\frac{(4n+2l+3)}{l_c^3}\right]^{1/2} \left[\frac{(1-y^2)}{\varepsilon_{nl}\zeta}\right]^{\pm 1/2} y^l P_n^{(l+1/2,0)}(1-2y^2) \\ \times Y_{lm}(\theta,\phi), \qquad (22)$$

where $l_c = (2 \mu/M \omega^2)^{1/2}$ is the size of the condensate. The spectrum (21) coincides with that found by Stringari [9] from the analysis of the density fluctuations in the hydrodynamic approach.

In the nonsymmetric case with $\omega_1 \neq \omega_2 \neq \omega_3$, the operator \hat{G} is invariant under the inversion of any of the three spatial coordinates. Therefore, the polynomials W determined by Eq. (17) can be labeled by the corresponding parities $\mathcal{P}_i = [\pm, \pm, \pm]$. Another quantum number is the order N of the polynomial W. For even N the function W contains the powers of y equal to $N, N-2, \ldots, 0$, and for odd N the powers are equal to $N, N-2, \ldots, 1$.

In fact, there are only two independent parities, since $\Pi_i \mathcal{P}_i = (-1)^N$. The first few eigenstates can easily be found. For N=1 we have three eigenstates describing the condensate center-of-mass oscillations with the trap frequencies. Accordingly, there are three eigenfunctions $W \propto y_i$ with parities $\mathcal{P}_i = [-]$. The corresponding eigenfrequencies are $\Omega = \overline{\omega}\varepsilon = \omega_i$. In the case of N=2 we again obtain three eigenstates corresponding to the condensate center-of-mass oscillations. The eigenfunctions are $W \propto y_i y_j$ $(i \neq j)$, the parities $\mathcal{P}_i = \mathcal{P}_j = [-]$, and the eigenfrequencies $\Omega = \sqrt{\omega_i^2 + \omega_j^2}$. In addition, there are three eigenstates with N=2 and parities $\mathcal{P}_i = [+]$ for all *i*. They correspond to the quadrupole oscillations of the condensate, the center of mass being at rest. The eigenfunctions can be written as

$$W \propto 1 + \sum_{i=1}^{3} b_i (\overline{\omega} / \omega_i)^2 y_i^2.$$

There are three different sets of coefficients b_i corresponding to the three eigenfrequencies Ω determined by the secular equation det[S]=0, where S is the 3×3 matrix

$$S_{ij} = 1 + (2 - \Omega^2 / \omega_i^2) \,\delta_{i,j} \,.$$

The coefficients b_i are determined by the system of three linear equations. The first one is $\sum_{i=1}^{3} b_i + (\Omega^2 / \overline{\omega}^2) = 0$. The

two other equations can be any of the three linearly dependent equations $\sum_{i=1}^{3} S_{ii} b_i = 0$.

For cylindrically symmetric traps $(\omega_1 = \omega_2 = \omega_{\rho}, \omega_3)$ $=\omega_z$) the projection of the orbital angular momentum on the z axis, m, is a conserved quantity. The eigenstates of the excitations can be labeled by the quantum numbers N, m and the axial parity \mathcal{P}_{7} . The radial parity describing the behavior of the eigenfunctions with respect to simultaneous inversion of the two radial coordinates is [+] for even m and [-] for odd m. The polynomials W can be represented in the form $W = \rho^{|m|} B_{nm}(\rho, z) \exp(im\phi)$, where ρ and z are the dimensionless axial and radial coordinates, and B_{nm} polynomials of power n = N - m. Each term of the polynomial B_{nm} has the form $z^{n_z} \rho^{n_\rho}$, where n_z and n_ρ are positive integers. The sum $n_z + n_\rho$ takes the values 0,2, ..., *n* for even *n*, and 1,3, ..., *n* for odd n. The integer n_{ρ} is even, n_z being even for even n $(\mathcal{P}_z = [+])$, and odd for odd n $(\mathcal{P}_z = [-])$. The polynomials $B_{nm}(\rho,z)$ and eigenenergies $E_{nm} = \hbar \Omega_{nm}$ can be found from the equation

$$\left[(1-\rho^2-z^2) \left(\frac{\partial^2}{\partial \rho^2} + \frac{(2|m|+1)}{\rho} \frac{\partial}{\partial \rho} + \beta^2 \frac{\partial^2}{\partial z^2} \right) - 2 \left(\rho \frac{\partial}{\partial \rho} + \beta^2 \frac{\partial^2}{\partial z^2} \right) + \beta^2 \frac{\partial^2}{\partial z} + 2 \left(\frac{\Omega_{nm}^2}{\omega_{\rho}^2} - m \right) \right] B_{nm}(\rho,z) = 0, \quad (23)$$

which follows directly from Eq. (17). The quantity $\beta = \omega_z / \omega_0$ is the ratio of the axial to radial frequency.

At given *m* and *n* the number of eigenmodes k = (n + 2)/2 for even *n*, and k = (n + 1)/2 for odd *n*. The eigenenergies can be found from the *k*th order secular equation det[*S*]=0, where *S* is the $k \times k$ matrix (i, j = 1, 2, ..., k):

$$S_{ij} = \left(\frac{\Omega_{nm}^2}{\omega_{\rho}^2} - |m|\right) \delta_{ij} - 2(k-j)(k-i+|m|+1)(\delta_{ij}+\delta_{i-1,j}) -\beta^2 \{ [2i-1-(-1)^n](2i-1)\delta_{ij}/2 +i[2i-(-1)^n]\delta_{i+1,j} \}.$$
(24)

For n=0 ($|m| \ge 1$) we have purely radial oscillations, with $B_{0m} = \text{const}$ and $\Omega_{0m} = \sqrt{|m|} \omega_{\rho}$. The case n=1 corresponds to the radial oscillations, in combination with the axial oscillations of the center of mass of the condensate. Here we have $B_{1m} \propto z$ and $\Omega_{1m} = \sqrt{|m|} \omega_{\rho}^2 + \omega_z^2$. In both cases the coupling between the radial and axial motion is absent, and the condensate frequencies Ω_{0m} and Ω_{1m} are the same as those for a classical gas in the hydrodynamic regime (see [16,17]).

For $n \ge 2$ the coupling between the radial and axial degrees of freedom becomes important, and the condensate oscillation frequencies will be different from the frequencies of a classical hydrodynamic gas. If n=2 there are two coupled shape oscillations of the condensate with frequencies Ω_{2m}^{\pm} given by

$$\frac{\Omega_{2m}^{\pm}}{\omega_{\rho}} = [2|m| + 2 + \frac{3}{2}\beta^{2} \\ \pm \sqrt{(|m| + 2 - \frac{3}{2}\beta^{2})^{2} + 2\beta^{2}(|m| + 1)}]^{1/2}.$$
 (25)

In the simplest case of m=0, Eq. (25) gives the frequencies of the quadrupole shape oscillations of the condensate. The

frequencies Ω_{20}^{\pm} and the frequency of quadrupole radial oscillations Ω_{02} were found in the hydrodynamic approach in [9]. They were also obtained in [15] by considering the condensate evolution under a weak modulation of the trap frequencies, in [16] from the Hamiltonian of the scaling dynamics, and in [13] on the basis of a variational approach. The frequencies Ω_{02} and Ω_{20}^{-} were measured in the experiment of Jin *et al.* [4] for $\beta = \sqrt{8}$ and calculated numerically for this trapping geometry in [10]. The frequencies Ω_{20}^{\pm} were found in the experiment of Mewes *et al.* [7] for $\beta = 0.08$.

For n=3 we have two coupled-shape oscillations, which are now also coupled to the oscillations of the center of mass of the condensate. In this case we obtain

$$\frac{\Omega_{3m}^{\pm}}{\omega_{\rho}} = [2|m| + 2 + \frac{7}{2}\beta^{2} \\ \pm \sqrt{(|m| + 2 - \frac{5}{2}\beta^{2})^{2} + 6\beta^{2}(|m| + 1)}]^{1/2}.$$
 (26)

Interestingly, for certain values of the projection of the orbital angular momentum *m*, we find an accidental degeneracy in the spectrum of excitations. The simplest example concerns the frequencies $\Omega_{1m} = \omega_{\rho} \sqrt{|m| + \beta^2}$ and Ω_{2m} . As follows from Eq. (25), $\Omega_{2m}^- = \Omega_{1m}$ for the projection *m* satisfying the condition

$$\beta^2 = |m| + 3 \tag{27}$$

and, accordingly, integer $\beta^2 \ge 3$. For $\beta = \sqrt{3}$ we have m = 0, i.e., the frequency of quadrupole shape oscillations Ω_{20}^- coincides with the frequency of axial oscillations Ω_{10} . In the trapping geometry of Jin *et al.*, where $\beta = \sqrt{8}$, Eq. (27) gives |m| = 5.

Although the condensate frequencies Ω_{2m} do not significantly differ from those for a classical gas in the hydrodynamic regime (the difference does not exceed 10%; for m = 0 see [16]), the accidental deeperacy determined by Eq.

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(27) is characteristic only for the condensate. In fact, this equation corresponds to the accidental degeneracy only in the limit $\zeta \rightarrow 0$. The non-Thomas-Fermi corrections, in particular those associated with the existence of Ψ_0 and the condensate excitations outside the Thomas-Fermi spatial region $y^2 < 1$, result in the extra splitting $\delta \Omega \sim \zeta \Omega_{1m}$ between the condensate eigenfrequencies Ω_{1m} and Ω_{2m} . For realistic values $\zeta \sim 0.1$, such as those achieved in the experiments of Jin *et al.* [8], $\delta \Omega$ is already comparable to the difference of the condensate frequency Ω_{2m} from Ω_{2m} of a classical hydrodynamic gas. It is important, however, that the splitting $\delta \Omega$ can be compensated by a slight change of β from that determined by Eq. (27), inducing the same splitting of the opposite sign between the Thomas-Fermi condensate frequencies Ω_{1m} and Ω_{2m} .

The presence of the accidental degeneracy can strongly influence the picture of the condensate oscillations. The coupling between the degenerate modes is provided by the interaction terms in the Hamiltonian (1), which are proportional to $\hat{\Psi}'^3$ and $\hat{\Psi}'^4$ and omitted above in the derivation of the Bogolyubov–de Gennes equations. Therefore, deriving only one of the degenerate modes, it is feasible to expect the appearance of oscillations representing a superposition of the two modes. This phenomenon ensures a clear distinction between the condensate oscillations and the oscillations of a classical hydrodynamic gas and, hence, can be a signature of BEC for the gas in the hydrodynamic regime.

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