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## LETTER TO THE EDITOR

## Comparison of mean-field theories for vortices in trapped Bose–Einstein condensates

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### Abstract

We compute structures of vortex configurations in a harmonically trapped Bose–Einstein condensed atom gas within three different gapless self-consistent mean-field theories. Outside the vortex core region, the density profiles for the condensate and the thermal gas derived from the Hartree–Fock–Bogoliubov–Popov theory are found to differ by only a few per cent from those derived from two of its recently proposed gapless extensions. In the core region, however, the differences between the density profiles are substantial. The structural differences are reflected in the energies of the quasiparticle states localized near the vortex core. In particular, the predictions for the energy of the lowest quasiparticle excitation derived from the theoretical models investigated differ considerably.

The landmark experiments realizing Bose–Einstein condensation in dilute atomic gases [1] have sparked off vigorous investigation of the physical properties of these novel quantum fluids. Due to the weak interactions, such systems are rare examples of interacting quantum fluids amenable to quantitative microscopic analysis, and thus provide unique possibilities for testing the fundamental principles and theories of many-body quantum physics. Theoretical approaches yield several quantities, such as density profiles for the condensate and the thermal gas component, stability estimates, specific heats, and properties of various propagating sound modes, to be compared with experiments. Experiments also yield detailed information on the energies of the individual excitation modes of these systems [2]. Such information provides the most direct and stringent tests for the accuracy of different theoretical approaches, as compared to the above-mentioned ‘collective’ quantities which depend on the excitation spectrum as a whole.

The Bogoliubov equations [3] are a widely used starting point for computing the excitation spectra for dilute Bose–Einstein condensates (BECs). They can be seen as eigenmode equations for the condensate described by the Gross–Pitaevskii equation [4], neglecting effects of the thermal, noncondensed gas component in the system. The Hartree–Fock–Bogoliubov (HFB) theory [5] takes self-consistently into account the condensate and the thermal gas

densities, as well as the lowest-order anomalous average of the boson field. However, it is plagued by an unphysical gap in the excitation spectrum, which violates Goldstone's theorem and invalidates its use in predicting the lowest collective-mode excitation frequencies. Goldstone's theorem can be restored by neglecting the anomalous average mean field in the HFB formalism. This yields the gapless Popov version of the HFB theory [6]. At low temperatures, predictions based on the Popov approximation (PA) for the lowest excitation frequencies of irrotational condensates are in good agreement with experimental results, but at temperatures  $T \gtrsim T_{\text{BEC}}/2$  ( $T_{\text{BEC}}$  denotes the critical temperature of condensation) deviations become apparent [7]. The main inadequacies of the PA are that it neglects the effects of the background gas on atomic collisions and the dynamics of the thermal gas component. As an improvement designed to overcome the first limitation within a computationally manageable formalism, the so-called G1 and G2 approximations have been suggested [8, 9]. They are gapless mean-field theories which take into account effects of the medium on atomic collisions by allowing the interaction couplings to depend on the correlation mean fields in a self-consistent manner. The two versions are based on different approximations for the momentum dependence of the full many-body  $T$ -matrix in the homogeneous gas limit, and their precision for inhomogeneous systems remains to be investigated.

To assess the accuracy of the above-mentioned gapless HFB-type approximations, the predictions that they lead to for the excitation frequencies of irrotational, harmonically trapped atomic BECs have been computed and compared with experimental results [7, 8, 10–12]. For temperatures  $T \lesssim T_{\text{BEC}}/2$ , the predictions from the PA, and the G1 and G2 approximations for the lowest excitation frequencies differ by only a few per cent [8, 9]. For higher temperatures, the differences are larger and exceed the experimental uncertainty estimates for measurements, but none of the theories agrees satisfyingly with experiments [8]. However, in this temperature range the dynamics of the thermal gas component, which these approximations do not take into account, is expected to have an increasingly important influence on the excitation eigenmodes. Consequently, results for irrotational condensates remain somewhat inconclusive in determining the validity of these theories.

Recently, vortex states in dilute atomic BECs have been experimentally realized [13]. Furthermore, by observing the precession of vortices, the energy of the lowest excitation, the so-called lowest core-localized state (LCLS), has been measured [14]. Interestingly enough, the experimental results for this energy agree well with the Bogoliubov approximation [15], while they definitely disagree with the picture given by the self-consistent mean-field theories: the latter predict the energy of the precession mode to be positive w.r.t. the condensate state [16, 17], but experiments imply negative energies. We suggest that this puzzling fact could be due to incomplete thermalization of the (moving) vortex and/or the limitations of the quasi-stationary, i.e., adiabatic HFB formalism in describing time-dependent phenomena. The adiabatic approximation essentially fails if the kinetic rates of the system exceed frequency separations of the excitations. Recently, we have shown that the requirement of adiabaticity leads to a criterion for the velocity of the moving vortex, which is violated in the precession observations made so far [18]. However, if the precession radii—and thus the velocities—of the vortices could be reduced, or the physical parameter values appropriately adjusted in order for the system to better fulfil the criteria for adiabaticity and thermalization, one should be able to meaningfully compare experimental data with the predictions of the self-consistent equilibrium theories for the vortex states.

In this letter, we present results of computations for the structures and excitation frequencies of vortex states within the G1 and the G2 approximations, and compare them with the previously computed predictions from the Popov approximation [16, 17]. Outside the vortex core region, the density profiles for the condensate and the thermal gas component

derived from the PA, and G1 and G2 approximations are found to differ by only a few per cent. However, in the core region the differences are considerably larger. This is reflected in substantial differences in the energy of the LCLS, which is localized in the core region.

The gapless HFB-type theories considered in this letter can be expressed in the form of the generalized Gross–Pitaevskii (GP) equation [5, 9]

$$[\mathcal{H}_0(\mathbf{r}) + U_c(\mathbf{r})|\phi(\mathbf{r})|^2 + 2U_e(\mathbf{r})\rho(\mathbf{r})]\phi(\mathbf{r}) = \mu\phi(\mathbf{r}) \quad (1)$$

for the condensate wavefunction  $\phi(\mathbf{r})$ , and the eigenvalue equations

$$\mathcal{L}(\mathbf{r})u_q(\mathbf{r}) + U_c(\mathbf{r})\phi^2(\mathbf{r})v_q(\mathbf{r}) = E_q u_q(\mathbf{r}) \quad (2a)$$

$$\mathcal{L}(\mathbf{r})v_q(\mathbf{r}) + U_c(\mathbf{r})\phi^{*2}(\mathbf{r})u_q(\mathbf{r}) = -E_q v_q(\mathbf{r}) \quad (2b)$$

for the quasiparticle amplitudes  $u_q(\mathbf{r})$ ,  $v_q(\mathbf{r})$ , and eigenenergies  $E_q$ . In equation (1), above,  $\mathcal{H}_0(\mathbf{r}) = -\hbar^2\nabla^2/2m + V_{\text{trap}}(\mathbf{r})$  is the bare single-particle Hamiltonian for atoms of mass  $m$  confined by a harmonic trapping potential  $V_{\text{trap}}(\mathbf{r}) = \frac{1}{2}m(\omega_r^2 r^2 + \omega_z^2 z^2)$  expressed in cylindrical coordinates  $\mathbf{r} = (r, \theta, z)$ . Furthermore,  $\mu$  denotes the chemical potential,  $\rho(\mathbf{r})$  is the noncondensate density, and  $\mathcal{L}(\mathbf{r}) \equiv \mathcal{H}_0(\mathbf{r}) - \mu + 2U_c(\mathbf{r})|\phi(\mathbf{r})|^2 + 2U_e(\mathbf{r})\rho(\mathbf{r})$ . The coupling functions  $U_c(\mathbf{r})$  and  $U_e(\mathbf{r})$  specify the approximation: in the Popov version  $U_c(\mathbf{r}) = U_e(\mathbf{r}) \equiv g$ , where the coupling constant  $g$  is related to the s-wave scattering length  $a$  by  $g = 4\pi\hbar^2 a/m$ . In the G1 approximation,  $U_e(\mathbf{r}) \equiv g$  and  $U_c(\mathbf{r}) = g[1 + \Delta(\mathbf{r})/\phi^2(\mathbf{r})]$ , where  $\Delta(\mathbf{r})$  is the anomalous average of two Bose field operators, and in the G2 approximation,  $U_e(\mathbf{r}) = U_c(\mathbf{r}) = g[1 + \Delta(\mathbf{r})/\phi^2(\mathbf{r})]$ . Finally, the self-consistency equations:

$$\rho(\mathbf{r}) = \sum_q [(|u_q(\mathbf{r})|^2 + |v_q(\mathbf{r})|^2)n(E_q) + |v_q(\mathbf{r})|^2] \quad (3)$$

$$\Delta(\mathbf{r}) = \sum_q [2u_q(\mathbf{r})v_q^*(\mathbf{r})n(E_q) + u_q(\mathbf{r})v_q^*(\mathbf{r})] \quad (4)$$

where  $n(E_q) = (\epsilon^{E_q/k_B T} - 1)^{-1}$  is the Bose distribution function (the chemical potential is set equal to the condensate eigenenergy—for the parameter values used in the computations, the effect of this approximation is negligible), relate the noncondensate density and the anomalous average to the positive-norm quasiparticle eigensolutions of equations (2a). The expression for the anomalous average is ultraviolet divergent, and we renormalize it by subtracting the last, only implicitly temperature-dependent terms from the sum of equation (4). This renormalization scheme neglects the difference between the two- and the many-body  $T$ -matrices, but for dilute gases the corrections are vanishingly small [19].

In this letter we consider axisymmetric single-quantum vortex states of the form  $\phi(\mathbf{r}) = \phi(r)e^{i\theta}$ , thus neglecting possible bending of the vortex [20]. Furthermore, we restrict consideration to the case  $\omega_z = 0$ , which implies the system to be homogeneous in the axial direction. However, the qualitative results concerning especially the substantial relative differences between the approximations in the lowest excitation energy are expected to remain valid also for systems with  $\omega_z > 0$ .

In accordance with the translational symmetry in the axial direction, we impose periodic boundary conditions at  $z = \pm L/2$ . On substituting in the *ansatz*

$$u_q(\mathbf{r}) = u_q(r)e^{iq_z(2\pi/L)z + i(q_\theta + 1)\theta} \quad (5a)$$

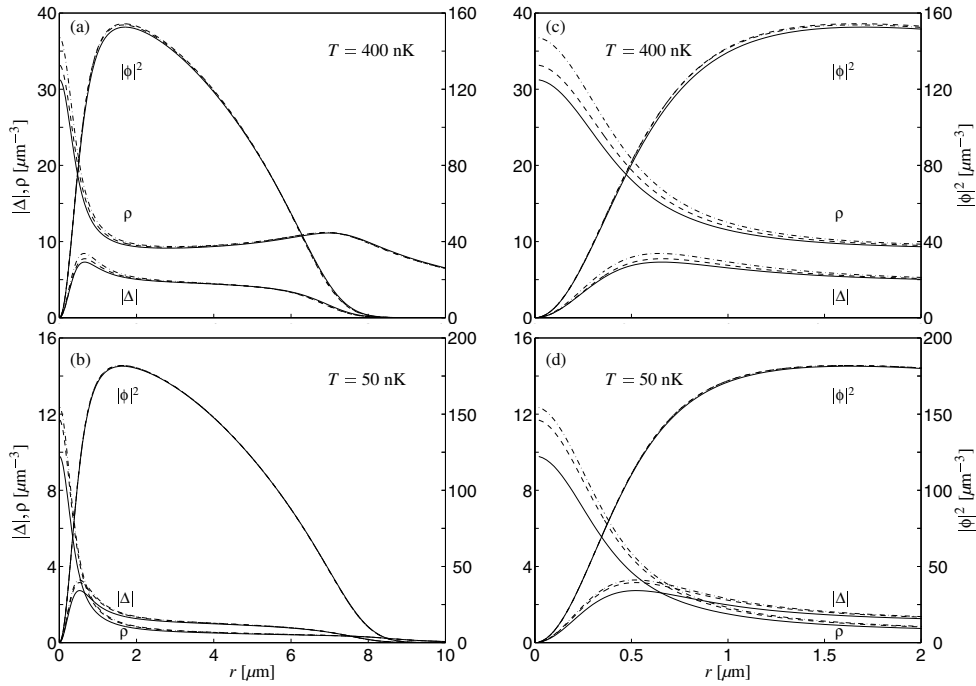
$$v_q(\mathbf{r}) = v_q(r)e^{iq_z(2\pi/L)z + i(q_\theta - 1)\theta} \quad (5b)$$

where  $q_\theta$  and  $q_z$  are integer quantum numbers, equations (2a) reduce to radial equations. We discretize them with a high-order finite-difference method and solve the consequent matrix eigenvalue problem by using an Arnoldi method implemented in the ARPACK (<http://www.caam.rice.edu/software/ARPACK/>) subroutine libraries [17]. The nonlinear

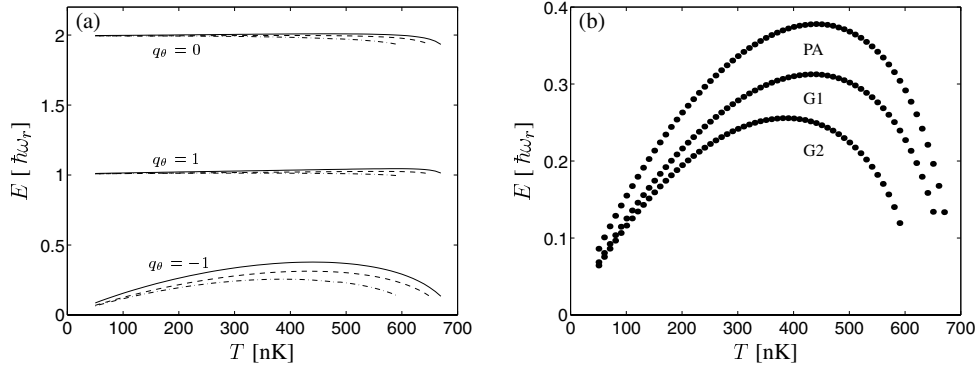
Gross–Pitaevskii equation is solved using a real-space discretization and iterative relaxation methods. Finally, self-consistency is achieved by iteration: using the solutions of equations (1) and (2a) corresponding to a given total number of particles, new mean-field potentials are computed from the self-consistency equations, and the procedure is repeated until convergence is achieved. We solve quasiparticle states explicitly up to an energy  $E_c$ , and compute the contribution to the mean-field potentials from the states above  $E_c$  by using a semiclassical local density approximation described in reference [11]. This method allows one to use rather small values for  $E_c$  with excellent accuracy, thus essentially improving the computational efficiency. In order to stabilize the iteration, we use under-relaxation in updating the mean-field potentials.

To facilitate comparison with previously presented results for the Popov approximation, the physical parameter values for the gas and the trap were chosen to be the same as those in reference [16]. We modelled sodium gas with the atomic mass  $m = 3.81 \times 10^{-26}$  kg and the scattering length  $a = 2.75$  nm in a trap with the radial frequency  $\nu_r = \omega_r/2\pi = 200$  Hz. The density of the gas was determined by treating  $N = 2 \times 10^5$  atoms per length  $L = 10 \mu\text{m}$  in the axial direction. Altogether, these values yield the condensation temperature  $T_{\text{BEC}} \approx 0.8 \mu\text{K}$ .

Figures 1 and 2 present results of our computations for axisymmetric single-quantum vortex states. The density profiles for the condensate, the noncondensate, and the anomalous average are displayed in figure 1 at temperatures  $T = 50$  nK and 400 nK. Outside the vortex core region, the differences between the density profiles derived from the PA, and G1 and G2



**Figure 1.** Density profiles of the vortex state for the condensate ( $|\phi|^2$ ), thermal gas component ( $\rho$ ), and anomalous average ( $|\Delta|$ ) in the PA (solid), G1 approximation (dashed), and G2 approximation (dashed-dotted) at temperatures (a)  $T = 400$  nK and (b)  $T = 50$  nK. Axes for the values of  $\rho$  and  $|\Delta|$  are on the left-hand sides, and for  $|\phi|^2$  on the right-hand sides. Panels (c) and (d) display the vortex core region, where the differences between the density profiles derived from the various approximations are substantially larger than further from the vortex axis.



**Figure 2.** (a) Energies of the lowest excitation modes with angular momentum quantum numbers  $q_\theta = -1, 0,$  and  $1$  in the PA (solid), G1 approximation (dashed), and G2 approximation (dashed-dotted) as functions of temperature. The  $q_\theta = -1$  state is the so-called lowest core-localized state (LCLS), and the  $q_\theta = 1$  excitation is the Kohn mode. (b) The temperature dependence of the energy of the LCLS within the PA, G1 approximation, and G2 approximation. Note the substantial relative differences between the energies derived from the different theories.

approximations are at most a few per cent at temperatures  $T \lesssim T_{\text{BEC}}/2$ . In the core region, however, the differences are considerably larger. The total density of the gas is approximately 20% larger on the vortex axis in the G2 approximation than within the PA. This squeezing behaviour is associated with the ‘softening’ of the repulsive effective interaction in the core region due to many-body effects [9].

The differences between the core densities derived using the various approximations also suggest differences in the energies of the quasiparticle excitations localized in the core region. Figure 2 displays the energies of three such states, the lowest excitations with angular momentum quantum numbers  $q_\theta = -1, 0,$  and  $1$ , as functions of temperature. For the G1 and G2 approximations, the increased core densities are compensated by smaller effective couplings, and the shifts in the excitation energies are generally only a few per cent for temperatures  $T \lesssim T_{\text{BEC}}/2$ ; at higher temperatures the softening effect of the interaction becomes more pronounced [9, 12], also increasing the shifts in the excitations. However, the lowest Kelvin mode (consisting of the lowest  $q_\theta = -1$  excitations) state, the LCLS, is especially sensitive to the structure of the core region. The differences between the energies of the LCLS derived from the approximations are 25–40% even at temperatures for which the predictions from the PA for the excitation frequencies of irrotational condensates differ by less than 5% from the experimental data. In addition, the temperature dependence of the LCLS is found to be much stronger than for the other states. In fact, the lowest excitation energy vanishes in the zero-temperature limit for all the approximations [17]; the remainder of the spectrum is essentially temperature independent, except in the vicinity of  $T_{\text{BEC}}$ . The state displayed in figure 2 with  $q_\theta = 1$  is the Kohn mode, which should have the exact energy  $E = \hbar\omega_r$  according to Kohn’s theorem for parabolic confinement [21]. Kohn’s theorem is satisfied to an accuracy of 1–6% for all the approximations, suggesting that dynamical effects of the thermal gas component are small in the temperature range studied.

In conclusion, we argue that future measurements of the lowest excitation frequencies of the vortex states could provide stringent tests for the validity of the mean-field theories considered. In particular, they could be used to estimate the degree to which the approximations for the many-body  $T$ -matrices based on the homogeneous limit remain valid for highly inhomogeneous systems.

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