A nonlinear dynamics approach to Bogoliubov excitations of Bose-Einstein condensates

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Abstract. We assume the macroscopic wave function of a Bose-Einstein condensate as a superposition of Gaussian wave packets, with time-dependent complex width parameters, insert it into the mean-field energy functional corresponding to the Gross-Pitaevskii equation (GPE) and apply the time-dependent variational principle. In this way the GPE is mapped onto a system of coupled equations of motion for the complex width parameters, which can be analyzed using the methods of nonlinear dynamics. We perform a stability analysis of the fixed points of the nonlinear system, and demonstrate that the eigenvalues of the Jacobian reproduce the low-lying quantum mechanical Bogoliubov excitation spectrum of a condensate in an axisymmetric trap.

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INTRODUCTION

It is well known that at sufficiently low temperatures the Gross-Pitaevskii equation (GPE) [1], a nonlinear Schrödinger equation for the macroscopic wave function, provides an accurate description of the dynamics of dilute trapped Bose-Einstein condensates for both the ground state and the excitation spectrum. For a condensate in a trap the GPE reads, in appropriately scaled units,

$$\left[-\Delta+\gamma_x^2x^2+\gamma_y^2y^2+\gamma_z^2z^2+8\pi a|\psi(\boldsymbol{r},t)|^2\right]\psi(\boldsymbol{r},t)=\mathrm{i}\frac{\partial}{\partial t}\psi(\boldsymbol{r},t). \tag{1}$$

Here a is the s-wave scattering length corresponding to the short-range contact interaction between the condensate atoms, and $\gamma_x,\gamma_y,\gamma_z$ are the frequencies of the traps confining the condensate in the three spatial directions. Because of its nonlinearity, the GPE can in general only be solved numerically, e.g. by imaginary time evolution (cf., e.g., [2]).

A full-fledged alternative to numerical quantum calculations is a variational approach [3] in which the trial functions are superpositions of N different Gaussians

$$\Psi(\mathbf{r})=\sum_{k=1}^{N}\mathrm{e}^{\mathrm{i}\left(a_x^k(t)\;x^2+a_y^k(t)\;y^2+a_z^k(t)\;z^2+\gamma^k(t)\right)}\equiv\sum_{k=1}^{N}g^k(\mathbf{y}^k(t),\mathbf{r})$$

with $3N$ complex width parameter functions $\boldsymbol{a}^k(t)$ and N functions $\gamma^k(t)$ which give the weights and phases of the individual Gaussians. Applying the Dirac-Frenkel variational principle [4, 5], i.e. requiring $||\mathrm{i}\phi(t)-H\Psi(t)||^2$ to be minimum with respect

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to the choice of ϕ, and afterwards setting $\phi = \dot{\psi}$, leads to equations of motion for the variational parameters which formally can be written

$$K\dot{\boldsymbol{\lambda}} = -\mathrm{i}\boldsymbol{h} \text{ with } K = \left\langle \frac{\partial \psi}{\partial \boldsymbol{\lambda}} \middle| \frac{\partial \psi}{\partial \boldsymbol{\lambda}} \right\rangle, \boldsymbol{h} = \left\langle \frac{\partial \psi}{\partial \boldsymbol{\lambda}} \middle| H \middle| \psi \right\rangle, \tag{2}$$

where $\boldsymbol{\lambda}$ stands for all variational parameters. Stationary solutions are then the fixed points of the equations of motion.

This method has been successfully applied to the description of Bose-Einstein condensates. Even for condensates with long-range interactions (monopolar and dipolar), in addition to the short-range contact interaction, the method leads to highly accurate results for energies and wave functions [6, 7, 8]. For example it well reproduces structured ground states that can appear in condensates of dipolar atoms [9] close to collapse, and which first had been predicted numerically [10]. The method has also successfully been applied to the dynamics of anisotropic solitons in dipolar Bose-Einstein condensates [11], and interacting multi-layer stacks of such condensates [12]. Moreover, the method is capable of giving access to regions of the space of solutions of the GPE that are difficult or impossible to investigate by conventional numerical calculations. In this way it was possible to reveal phenomena characteristic of nonlinear classical systems in the theory of Bose-Einstein condensates such as the appearance of bifurcations [8], exceptional points [13], and the transition from order to chaos [14].

In this paper we will address the two different concepts of stability that are involved in the two approaches. In the full quantum mechanical treatment the stability of Bose-Einstein condensates is investigated by calculating Bogoliubov excitations of the ground state. In the nonlinear dynamics approach stability is determined by calculating the eigenvalues of the Jacobian at the fixed points. Is there a relation between these eigenvalues and the frequencies of the quantum mechanical Bogoliubov excitations?

BOGOLIUBOV-DE GENNES EQUATIONS

We consider a Bose-Einstein condensate in an axisymmetric trap, i.e. in (1) only two trap frequencies, γ_z, γ_ρ appear. If $\psi_0(\mathbf{r})$ is the stationary solution of the GPE, with μ its chemical potential, the Bogoliubov ansatz for elementary excitations is

$$\psi(\mathbf{r},t) = \left[\psi_0(\mathbf{r}) + u(\mathbf{r})\mathrm{e}^{-\mathrm{i}\omega t} + v^*(\mathbf{r})\mathrm{e}^{\mathrm{i}\omega t}\right]\mathrm{e}^{-\mathrm{i}\mu t}. \tag{3}$$

Inserting this into (1) and linearizing in the perturbations u and v around the stationary solution yields the Bogoliubov-de Gennes (BDG) equations

$$\omega u(\mathbf{r}) = \left[-\Delta + \gamma_\rho^2\rho^2 + \gamma_z^2 z^2 - \mu + 16\pi a|\psi_0(\mathbf{r})|^2\right] u(\mathbf{r}) + 8\pi a\left(\psi_0(\mathbf{r})\right)^2 v(\mathbf{r}), \tag{4}$$

$$-\omega v(\mathbf{r}) = \left[-\Delta + \gamma_\rho^2\rho^2 + \gamma_z^2 z^2 - \mu + 16\pi a|\psi_0(\mathbf{r})|^2\right] v(\mathbf{r}) + 8\pi a\left(\psi_0^*(\mathbf{r})\right)^2 u(\mathbf{r}). \tag{5}$$

Because of the axial symmetry we can make the separation ansatz $u = \mathrm{e}^{\mathrm{i}m\varphi}u_m(\rho,z)$, $v = \mathrm{e}^{\mathrm{i}m\varphi}v_m(\rho,z)$, where $m = 0,1,2,\ldots$ is the azimuthal (angular momentum) quantum

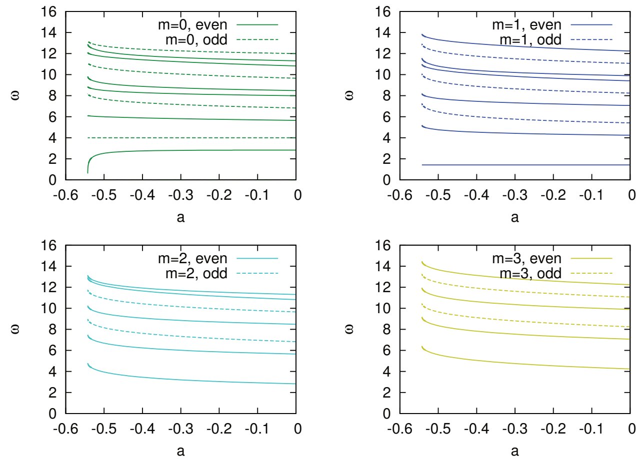

FIGURE 1. Frequencies of Bogoliubov excitations of the ground state of a BEC in an axisymmetric trap as functions of the scattering length for different values of the azimuthal quantum number m. The lowest lying modes are shown for each m. The trap frequencies chosen are $\gamma_\rho = 1/\sqrt{2}$, $\gamma_z = 2$.

number of the perturbation. Since the system is also invariant under reflections $z \to -z$, the excitation modes can also be classified according to their z-parity, even or odd. The equations were solved following a procedure described by Ronen et al. [15], which takes advantage of discrete Hankel-Fourier transforms to move between space and momentum space representations and uses the Arnoldi method to efficiently compute the low lying eigenvalues.

Figure 1 shows the results for the frequencies of low lying modes as functions of the scattering length for angular excitations with $m = 0, 1, 2$ and 3 for a pancake-shaped trap with $\gamma_\rho = 1/\sqrt{2}$, $\gamma_z = 2$. It can be seen that all eigenfrequencies are real over a wide range of the scattering length, which just confirms that the ground state is stable with respect to elementary excitations. At $a \approx -0.55$ the frequency of the lowest $m = 0$ mode turns negative, i.e. it is this mode which induces the collapse of the condensate at this scattering length.

COUPLED GAUSSIAN WAVE PACKETS

The variational ansatz for the wave function that respects the remaining symmetries of the systems, axial symmetry and z parity, is

$$\psi = \sum_m \mathrm{e}^{\mathrm{i}m\phi} \rho^{|m|} \sum_{p=0,1} z^p \left(\sum_{k=1}^{N} d_{m,p}^k \mathrm{e}^{-(A_\rho^k \rho^2 + A_z^k z^2 + p_z^k z + \gamma^k)} \right), \tag{6}$$

with

$$A_\rho^k = A_\rho^k(t),\; A_z^k = A_z^k(t),\; d_{m,p}^k = d_{m,p}^k(t) \in \mathbb{C}.$$

The factor z^p distinguishes states with even or odd z parity, $p = 0, 1$. For a fixed value of m we insert this ansatz into the time-dependent variational principle and derive the

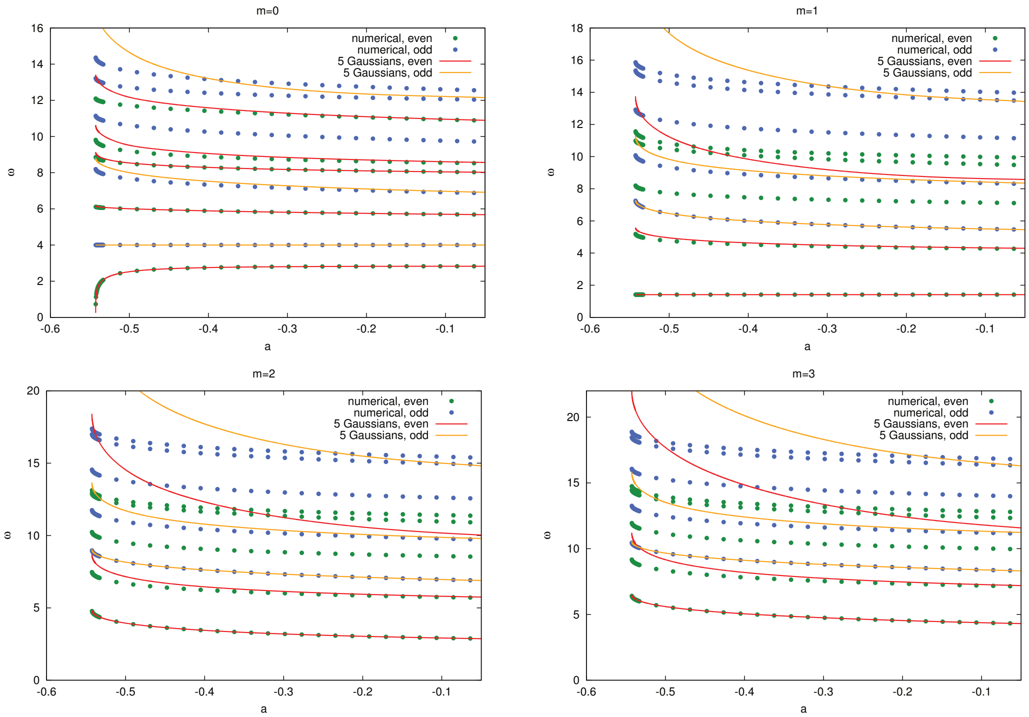

FIGURE 2. Comparison of the full-numerical Bogoliubov spectrum of a BEC in an axisymmetric trap with attractive contact interaction with the spectrum obtained from the variational ansatz with 5 coupled Gaussians for the azimuthal excitations with $m = 0, 1, 2, 3$. As in Fig. 1 the trap frequencies chosen are $\gamma_\rho = 1/\sqrt{2}$, $\gamma_z = 2$.

equations of motion for the variational parameters. The advantage of using Gaussians is that in calculating the energy functional all necessary integrals can be expressed analytically. The fixed points are then determined by a nonlinear root-search of the equations of motion. Finally the Jacobian is evaluated at the fixed points and diagonalized.

The results are shown in Fig. 2 where we compare the eigenvalue spectrum of the Jacobian calculated in dependence on the scattering length with the frequencies of the corresponding Bogoliubov excitations. One recognizes that in particular the eigenvalues of the lowest modes of each azimuthal excitation agree well with the eigenfrequencies of the Bogoliubov excitations. It is only close to the critical scattering length that small deviations appear. For the higher modes with eigenvalues of the Jacobian $\omega > 10$, only far away from the collapse point the variational and full-numerical results still approximately correspond to each other, and in the vicinity of the critical scattering length the Jacobi eigenvalues can reproduce the behavior of the Bogoliubov excitation eigenfrequencies only qualitatively.

We have also applied the variational ansatz to azimuthal excitations up to $m = 6$. The results for a fixed scattering length of $a = -0.4$ are presented in Fig. 3. One recognizes a very good agreement for the lowest modes in each m band, and small differences for the second-lowest modes.

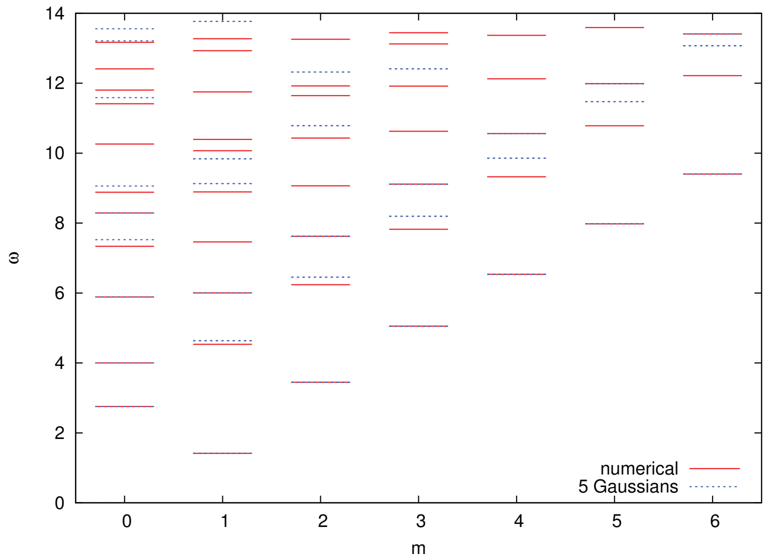

FIGURE 3. Comparison of both spectra as in Fig. 2, but here for a fixed scattering length of $a = -0.4$ and azimuthal excitations up to $m = 6$. For $m = 0$ the variational ansatz reproduces the Bogoliubov frequencies very well for the four lowest modes, and with only small deviations for the two lowest modes in the bands with $m > 0$.

CONCLUSIONS AND OUTLOOK

We have demonstrated that for condensates with attractive short-range interaction in an axisymmetric trap the eigenvalues of the Jacobian matrix calculated at the fixed point corresponding to the ground state in the variational ansatz (6) with coupled Gaussian wave packets *quantitatively* coincide with the eigenfrequencies of the lowest quantum mechanical Bogoliubov modes.

This is remarkable because it establishes a link between two completely different concepts of stability: On the one hand the quantum mechanical stability of a wave function with respect to elementary excitations, on the other hand the stability of a classical dynamical system at a fixed point with respect to small perturbations.

This finding is not restricted to condensates in axisymmetric traps. Kreibich et al. [16] have demonstrated that for condensates in radially symmetric trapping potentials there is also a good agreement between the quantum mechanical eigenfrequencies of the lowest Bogoliubov excitations and the eigenvalues of the Jacobian stability matrix. Their analysis is more involved since, to account for the spherical symmetry of the systems, the variational ansatz (6) has to be modified to include also spherical harmonics

$$\psi = \sum_{k=1}^{N} \left(1 + \sum_{(l,m)\neq(0,0)} d_{lm}^k Y_{lm}(\theta,\phi) r^l \right) \mathrm{e}^{-A_r^k r^2 - \gamma^k}. \tag{7}$$

The amplitudes d_{lm}^k of the spherical harmonics are additional variational functions of time, whose equations of motion must be obtained from the time-dependent variational principle, together with those for the variational functions entering the Gaussians. The fixed points again correspond to the stationary ground states.

The variational approach should also be extended to Bose condensates in which the atoms interact via long-range forces. The most prominent examples are condensates of atoms with a large magnetic moment such as ^{52}Cr [17], ^{164}Dy [18, 19], and other lanthanides [20], in which the dipole-dipole interaction is active.

As a model system with long-range interaction, monopolar condensates, with *gravity-like* attractive long-range interaction, have been proposed [21]. The interaction is induced by shining an appropriate arrangement of lasers on the condensate. Such condensates are unique in that they exhibit the phenomenon of self-trapping, without an external potential. They are of special theoretical interest since their investigation can serve as a useful guide to studies of the more complicated situation of Bose-Einstein condensates with the anisotropic dipole-dipole interaction. For example, the occurrence of exceptional points in Bose-Einstein condensates was first shown for the monopolar interaction [22] before it was also demonstrated to appear in dipolar condensates [23].

Kreibich et al. [16] have already looked at Bose-Einstein condensates with $1/r$ interaction in radially symmetric traps. They discovered that for self-trapped condensates a good agreement between the eigenvalues of the Jacobian and the eigenfrequencies of Bogoliubov excitations is present only for the very lowest modes, while the variational approach works less well for higher modes. The reason is that for condensates in a trap the confining radially symmetric harmonic potential dominates the properties of the system over a wide range of the scattering length, and the interactions quasi act as perturbations. Therefore, a variational ansatz in which the radial part is determined by Gaussians is very well adapted to describe the stationary solutions and their excitations.

On the other hand, for the special situation of a self-trapped monopolar condensate, the interactions alone determine the properties of the system. Asymptotically, for $r \to \infty$ the BDG equations assume the form of the Schrödinger equation of the hydrogen atom. Therefore for large r the solutions u and v assume the decaying shape of hydrogen wave functions $\propto \exp(-\alpha r)$, with some $\alpha > 0$. A variational ansatz with coupled Gaussians and spherical harmonics obviously is not well suited to reproduce this asymptotic behavior. However, as soon as a radially symmetric trap is switched on, the agreement between the quantum mechanical and the nonlinear dynamics excitations is present again also for the higher modes. We can therefore conclude that this agreement is of generic type, and should also be present for dipolar condensates. Investigations along this line are in progress.

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