Variational methods with coupled Gaussian functions for Bose-Einstein condensates with long-range interactions. I. General concept

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The variational method of coupled Gaussian functions is applied to Bose-Einstein condensates with long-range interactions. The time dependence of the condensate is described by dynamical equations for the variational parameters. We present the method and analytically derive the dynamical equations from the time-dependent Gross-Pitaevskii equation. The stability of the solutions is investigated using methods of nonlinear dynamics. The concept presented in this article will be applied to Bose-Einstein condensates with monopolar $1/r$ and dipolar $1/r^3$ interaction in the subsequent article [S. Rau *et al.*, Phys. Rev. A **82**, 023611 (2010)], where we will present a wealth of phenomena obtained using the ansatz with coupled Gaussian functions.

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I. INTRODUCTION

The experimental realization of Bose-Einstein condensates (BECs) with ^{52}Cr atoms [1,2], with a strong dipole-dipole interaction has given new impetus to theoretical investigations of BEC with long-range interactions.

The theoretical description of BECs in the dilute limit in the framework of the extended Gross-Pitaevskii equation (GPE) is well known. The derivation of the extended GPE from a many-particle Schrödinger equation is part of many textbooks on quantum mechanics or BECs [3]. For a long-range interaction of the form $W_{\mathrm{lr}}(\boldsymbol{r},\boldsymbol{r}') \propto |\boldsymbol{r}-\boldsymbol{r}'|^{\alpha}$, the time-dependent GPE can be brought into particle-number-scaled dimensionless form using appropriate units (for monopolar or dipolar condensates, see [4,5]) and reads

$$\left[-\Delta+\gamma_x^2x^2+\gamma_y^2y^2+\gamma_z^2z^2+8\pi a_{\mathrm{sc}}|\psi(\boldsymbol{r},t)|^2 + \int d^3\boldsymbol{r}'W_{\mathrm{lr}}(\boldsymbol{r},\boldsymbol{r}')|\psi(\boldsymbol{r}',t)|^2\right]\psi(\boldsymbol{r}) = i\frac{d}{dt}\psi(\boldsymbol{r},t). \quad (1)$$

The terms in Eq. (1) describe the short-range contact interaction between two particles, the s-wave scattering, $V_{\mathrm{sc}} = 8\pi a_{\mathrm{sc}}|\psi(\boldsymbol{r})|^2$, a harmonic model for external magnetic trapping of the condensate, $V_t = \gamma_x^2x^2+\gamma_y^2y^2+\gamma_z^2z^2$, and long-range interactions between two particles,

$$V_{\mathrm{lr}}(\boldsymbol{r}) = \int d^3\boldsymbol{r}'W_{\mathrm{lr}}(\boldsymbol{r},\boldsymbol{r}')|\psi(\boldsymbol{r}')|^2.$$

The mean-field energy reads

$$E_{\mathrm{mf}} = \langle\psi|-\Delta+V_t+(V_{\mathrm{sc}}+V_{\mathrm{lr}})/2|\psi\rangle. \quad (2)$$

So far, in most publications one of two methods for solving the GPE is used. The ground state for the GPE with long-range interaction in Eq. (1) is obtained by minimizing the energy functional (2) using different approaches.

The first method consists of numerical lattice calculations [6], either the minimization of the energy with conjugate gradients or imaginary time evolution of an initial wave function using the split-operator method and fast Fourier transform. The numerical calculations are, on the one hand, very accurate if they are carried out on sufficiently large grids. On the other hand, however, they may turn out to be laborious and may take a long computational time.

The second well-established method is to use a simple variational ansatz. A common ansatz is to assume a Gaussian-type wave function [7–11]. This technique makes it possible to gain physical insight, as it often provides qualitatively correct, although quantitatively inaccurate results. The extension and improvement of variational techniques for BECs with long-range interactions is the major challenge of this article.

We propose, as a third approach, an improved variational ansatz with coupled Gaussian functions. The method was originally proposed by Heller [12,13] to describe atomic and molecular quantum dynamics. Using the ansatz

$$\psi(\boldsymbol{x},t) = \sum_n \exp\{i[(\boldsymbol{x}-\boldsymbol{x}_{t,n})\boldsymbol{A}_{t,n}(\boldsymbol{x}-\boldsymbol{x}_{t,n}) + \boldsymbol{p}_{t,n}(\boldsymbol{x}-\boldsymbol{x}_{t,n})+\gamma_{t,n}]\}, \quad (3)$$

where the symmetric matrix $\boldsymbol{A}_{t,n}$, the vector $\boldsymbol{p}_{t,n}$, and the scalar $\gamma_{t,n}$ describe the width, momentum, and weight of the Gaussian wave packet, respectively, Heller approximated the dynamics of quantum wave packets following classical trajectories. The method was recently successfully applied to the dynamics of atoms in external fields [14,15] using up to $N = 100$ coupled functions.

We apply this method to BECs with long-range interactions using an ansatz with N coupled Gaussian functions centered at the origin, $\boldsymbol{x}_{t,n} = 0$, and with $\boldsymbol{p}_{t,n} = 0$, viz.,

$$\psi(\boldsymbol{r},t) = \sum_{k=1}^{N}\left[e^{i\gamma^k}\prod_{\alpha}\left(e^{ia_{\alpha}^kx_{\alpha}^2}\right)\right], \quad (4)$$

where $\alpha \in \{x,y,z\}$ for a BEC without symmetries, $\alpha \in \{\varrho,z\}$ for an axisymmetric, and $\alpha = r$ for a spherically symmetric BEC.

The ansatz in Eq. (4) is rather general and is not only able to describe condensates with spherical or axial symmetry, but also nonsymmetric condensates in arbitrary trap geometries or even anisotropic solitons [16,17]. The method is also well suited for long-range interactions because by its very nature it requires integrals over the entire wave function which show a similar behavior as the integrals for local interactions. Note that, as is typical for a Gaussian basis set, the individual Gaussian

functions in Eq. (4) are not orthogonal among each other. In this article we present the theoretical concept of the method and derive the necessary equations for arbitrary long-range interaction. For monopolar $(1/r)$ or dipolar $(1/r^3)$ interaction, selected results have already been presented in [18]. Results elaborated in more detail are subject of the subsequent article [19]. With the use of multiple Gaussians and thus an extended set of variational parameters, we are not only able to describe the stable ground state and the metastable stationary states, but can also identify the types of bifurcations where branches emerge or stability changes take place.

The article is organized as follows. In Sec. II we apply a time-dependent variational principle to the GPE (1) and obtain dynamical equations, which describe the time-dependence of the variational parameters. In Sec. III we evaluate the integrals that are needed to set up this nonlinear set of dynamical equations. In Sec. IV we present different methods for obtaining stationary solutions, and in Sec. V we investigate the stability of those states. Conclusions are given in Sec. VI.

II. TIME-DEPENDENT VARIATIONAL PRINCIPLE

The first variational principle for optimizing a variational wave function that comes to mind is minimizing the mean-field energy functional. For few variational parameters the analytical calculation is done easily, but it gets increasingly difficult if more variational parameters are included in the wave function. For a BEC with long-range interaction and more than three parameters, it turns out to be almost impossible to calculate all derivations analytically. Therefore, we will introduce a different approach based on the Dirac-Frenkel-McLachlan variational principle [20,21]. The application of this variational principle yields a set of differential equations for the parameters z of the trial wave function $\psi(t) = \psi(\boldsymbol{z}(t))$, where

$$\boldsymbol{z}(t) = (z_1(t), z_2(t), \ldots, z_M(t)) \tag{5}$$

is the vector consisting of all M variational parameters. The time dependence of a quantum system is described by the respective Schrödinger equation or GPE

$$H\psi(t) = i\frac{d}{dt}\psi(t). \tag{6}$$

The variational principle of McLachlan minimizes the difference between the left- and the right-hand side of the respective Schrödinger equation (6) with respect to the trial wave function,

$$I = ||i\dot{\phi}(t) - H\psi(t)||^2 \stackrel{!}{=} \min. \tag{7}$$

For any t, $\psi(t)$ is supposed to be fixed and given, and the quantity I is minimized by varying ϕ. Afterward, ϕ is set equal to $\phi = \dot{\psi}$. The time dependence of the trial wave function carries over to the time dependence of the variational parameters, $\psi(t) = \psi(\boldsymbol{z}(t))$. We consider variations of I in Eq. (7) with respect to ϕ,

$$\begin{aligned}\delta I &= \langle \delta\phi \,|\, \phi\rangle + \langle \phi \,|\, \delta\phi\rangle + i\langle \delta\phi \,|\, H\psi\rangle - i\langle H\psi \,|\, \delta\phi\rangle \\ &= \langle \delta\phi \,|\, \phi + iH\psi\rangle + \langle \phi - iH\psi \,|\, \delta\phi\rangle,\end{aligned} \tag{8}$$

where the variation of the time derivative of the wave function $\delta\phi$ carries over to variations of the parameters z,

$$|\delta\phi\rangle = |\delta\dot{\psi}(z,\dot{z})\rangle = \left|\frac{\partial\dot{\psi}}{\partial z}\delta z\right\rangle + \left|\frac{\partial\dot{\psi}}{\partial\dot{z}}\delta\dot{z}\right\rangle. \tag{9}$$

The first term vanishes, since we minimize I under the condition that $\psi(t)$ is fixed and therefore that all parameters z are fixed as well, and we obtain

$$|\delta\phi\rangle = \left|\frac{\partial}{\partial\dot{z}}\left(\frac{\partial\psi}{\partial z}\dot{z}\right)\delta\dot{z}\right\rangle = \left|\frac{\partial\psi}{\partial z}\delta\dot{z}\right\rangle. \tag{10}$$

We insert Eq. (10) in Eq. (8), set $\phi = \dot{\psi}$, and obtain as condition for the vanishing variation of I

$$\delta I = \left\langle \frac{\partial\psi}{\partial z}\delta\dot{z}\,\middle|\, \dot{\psi} + iH\psi\right\rangle + \left\langle \dot{\psi} - iH\psi\,\middle|\, \frac{\partial\psi}{\partial z}\delta\dot{z}\right\rangle = 0. \tag{11}$$

The variational parameters z are complex quantities and therefore the variations $\delta\dot{z}_k$ and $\delta\dot{z}_k^*$ for $k = 1,\ldots,M$ are independent. Therefore, both brackets of Eq. (11) have to vanish separately. This finally yields the equation

$$\left\langle \frac{\partial\psi}{\partial z}\,\middle|\, i\dot{\psi} - H\psi\right\rangle = 0, \tag{12}$$

which is easily transformed to an implicit dynamical set of equations $\boldsymbol{K}\dot{\boldsymbol{z}} = -i\boldsymbol{h}$ for the variational parameters with

$$\boldsymbol{K} = \left\langle \frac{\partial\psi}{\partial z}\,\middle|\, \frac{\partial\psi}{\partial z}\right\rangle, \quad \boldsymbol{h} = \left\langle \frac{\partial\psi}{\partial z}\,\middle|\, H\psi\right\rangle.$$

Up to this point there has been no specification of the trial wave function ψ or the Hamiltonian H. The variational principle can be applied to both linear and nonlinear Hamiltonians. In the following we apply the time-dependent variational principle (TDVP) to a trial wave function given as coupled Gaussian wave functions and derive dynamical equations for the variational parameters of each Gaussian.

A. Dynamical equations for condensates without symmetries

We choose a superposition of N Gaussians as a trial wave function,

$$\psi(\boldsymbol{r},t) = \sum_{k=1}^{N} g^k = \sum_{k=1}^{N} e^{i(a_x^k x^2 + a_y^k y^2 + a_z^k z^2 + \gamma^k)}. \tag{13}$$

The a_α^k for $\alpha \in \{x,y,z\}$ denote complex Gaussian "width" parameters in the three spatial directions and γ^k the complex amplitude and phase parameters. The system is described by the extended GPE (1) with the Hamiltonian brought to the scaled "natural" units for the respective long-range interaction,

$$\hat{H} = -\Delta + V_{\text{eff}}(\boldsymbol{r}), \tag{14}$$

where $V_{\text{eff}}(\boldsymbol{r}) = V_t(\boldsymbol{r}) + V_{\text{sc}}(\boldsymbol{r}) + V_{\text{lr}}(\boldsymbol{r})$ is the sum of the trapping, scattering, and long-range potential. We use Eq. (12) obtained from the TDVP for the complex variational parameters,

$$\boldsymbol{z} = \left(\gamma^1,\ldots,\gamma^N, a_x^1,\ldots,a_x^N, a_y^1,\ldots,a_y^N, a_z^1,\ldots,a_z^N\right), \tag{15}$$

and first calculate the time derivative $\dot{\psi}$ of the coupled Gaussian wave function. The derivation carries over to time

derivatives of the Gaussian width and the amplitude and phase parameters,

$$\frac{d}{dt}\sum_{k=1}^{N} g^k = \sum_{k=1}^{N} i\left(x^2\dot{a}_x^k + y^2\dot{a}_y^k + z^2\dot{a}_z^k + \dot{\gamma}^k\right)g^k. \quad (16)$$

Second, we apply the Laplace operator of the Hamiltonian in Eq. (14) in Cartesian coordinates,

$$-\Delta\psi = \sum_{k=1}^{N}\left\{-2i\left[a_x^k + a_y^k + a_z^k\right] + 4\left[\left(a_x^k\right)^2x^2 + \left(a_y^k\right)^2y^2 + \left(a_z^k\right)^2z^2\right]\right\}g^k, \quad (17)$$

and obtain the complete expression for the ket in Eq. (12),

$$i\dot{\psi} - H\psi = \sum_{k=1}^{N}\left(-\left\{x^2\dot{a}_x^k + y^2\dot{a}_y^k + z^2\dot{a}_z^k + \dot{\gamma}^k\right\} - \left\{V_{\mathrm{eff}}(\boldsymbol{r}) - 2i\left[a_x^k + a_y^k + a_z^k\right] + 4\left[\left(a_x^k\right)^2x^2 + \left(a_y^k\right)^2y^2 + \left(a_z^k\right)^2z^2\right]\right\}\right)g^k. \quad (18)$$

The sorting of Eq. (18) according to powers of the coordinates x,y,z results in a sum of products of a polynomial of second order and the Gaussian g^k,

$$i\dot{\psi} - H\psi = \sum_{k=1}^{N}\left[v_0^k + \frac{1}{2}\left(V_{2,x}^k x^2 + V_{2,y}^k y^2 + V_{2,z}^k z^2\right) - V_{\mathrm{eff}}(\boldsymbol{r})\right]g^k, \quad (19)$$

with the newly defined quantities

$$v_0^k = -\dot{\gamma}^k + 2i\left(a_x^k + a_y^k + a_z^k\right), \quad (20a)$$

$$\tfrac{1}{2}V_{2,\alpha}^k = -4\left(a_\alpha^k\right)^2 - \dot{a}_\alpha^k; \quad \alpha \in \{x,y,z\}. \quad (20b)$$

Now, we calculate the derivatives of $\psi = \sum_{l=1}^{N} g^l$ in Eq. (12) with respect to the variational parameters $\boldsymbol{z}$ in Eq. (15) for each $l = 1,\ldots,N$:

$$\frac{\partial\psi}{\partial\gamma^l} = ig^l, \quad \frac{\partial\psi}{\partial a_\alpha^l} = ix_\alpha^2 g^l; \quad \alpha \in \{x,y,z\}. \quad (21)$$

Finally, Eq. (12) results in the $4N$-dimensional system of equations

$$\left\langle \eta^2 g^l \middle| \sum_{k=1}^{N}\left[v_0^k + \frac{1}{2}\left(V_{2,x}^k x^2 + V_{2,y}^k y^2 + V_{2,z}^k z^2\right) - V_{\mathrm{eff}}(\boldsymbol{r})\right]g^k\right\rangle = 0, \quad (22)$$

with $l = 1,\ldots,N$ and $\eta = 1,x,y,z$, which can be sorted as

$$\sum_{k=1}^{N}\langle g^l \mid g^k\rangle v_0^k + \frac{1}{2}\sum_{k=1}^{N}\sum_{\alpha}\langle g^l|x_\alpha^2|g^k\rangle V_{2,\alpha}^k = \sum_{k=1}^{N}\langle g^l|V_{\mathrm{eff}}|g^k\rangle; \quad l = 1,\ldots,N;$$

$$\sum_{k=1}^{N}\langle g^l|x_\beta^2|g^k\rangle v_0^k + \frac{1}{2}\sum_{k=1}^{N}\sum_{\alpha}\langle g^l|x_\alpha^2x_\beta^2|g^k\rangle V_{2,\alpha}^k = \sum_{k=1}^{N}\langle g^l|x_\beta^2 V_{\mathrm{eff}}|g^k\rangle; \quad \beta \in \{x,y,z\}; \quad l = 1,\ldots,N, \quad (23)$$

where for a BEC without symmetries $\alpha,\beta \in \{x,y,z\}$. Equation (23) can be written in the form of a matrix equation,

$$\boldsymbol{M}\boldsymbol{v} = \boldsymbol{r}, \quad (24)$$

with the Hermitian, positive definite $4N \times 4N$ matrix $\boldsymbol{M}$,

$$\boldsymbol{M} = \begin{pmatrix} (1)_{lk} & (x^2)_{lk} & (y^2)_{lk} & (z^2)_{lk} \\ (x^2)_{kl} & (x^4)_{lk} & (x^2y^2)_{lk} & (x^2z^2)_{lk} \\ (y^2)_{kl} & (y^2x^2)_{kl} & (y^4)_{lk} & (y^2z^2)_{lk} \\ (z^2)_{kl} & (z^2x^2)_{kl} & (z^2y^2)_{kl} & (z^4)_{lk} \end{pmatrix}, \quad (25)$$

where all terms are $N \times N$ matrices for $k = 1,\ldots,N$ and $l = 1,\ldots,N$. As an example, the term $(x^2)_{lk}$ reads

$$(x^2)_{lk} = \begin{pmatrix} \langle g^{l=1}|x^2|g^{k=1}\rangle & \cdots & \langle g^{l=1}|x^2|g^{k=N}\rangle \\ \vdots & & \vdots \\ \langle g^{l=N}|x^2|g^{k=1}\rangle & \cdots & \langle g^{l=N}|x^2|g^{k=N}\rangle \end{pmatrix}. \quad (26)$$

The terms denoted $(y^2)_{lk}$,$(z^2)_{lk}$,$(x^2y^2)_{lk}$, . . . , are analogous to the example and obtained by replacing the x^2 with y^2, z^2, x^2y^2, . . . , respectively. The vectors $\boldsymbol{v}$ and $\boldsymbol{r}$ in Eq. (24) are

$$\boldsymbol{v} = \begin{pmatrix} v_0^k \\ \frac{1}{2}V_{2,x}^k \\ \frac{1}{2}V_{2,y}^k \\ \frac{1}{2}V_{2,z}^k \end{pmatrix}, \quad (27)$$

$$\boldsymbol{r} = \sum_{k=1}^{N}\begin{pmatrix} \langle g^l|V_{\mathrm{eff}}|g^k\rangle \\ \langle g^l|x^2V_{\mathrm{eff}}|g^k\rangle \\ \langle g^l|y^2V_{\mathrm{eff}}|g^k\rangle \\ \langle g^l|z^2V_{\mathrm{eff}}|g^k\rangle \end{pmatrix}, \quad (28)$$

where each entry is a vector of length N for $k = 1,\ldots,N$ and $l = 1,\ldots,N$, respectively.

By solving the definitions of $(v_0^k, \boldsymbol{V}_2^k)$ in Eq. (20) for the time derivatives of the Gaussian parameters, we obtain $4N$ dynamical equations for the Gaussian parameters $\boldsymbol{z}$,

$$\dot{\gamma}^k = 2i\left(a_x^k + a_y^k + a_z^k\right) - v_0^k, \quad (29a)$$

$$\dot{a}_\alpha^k = -4\left(a_\alpha^k\right)^2 - \tfrac{1}{2}V_{2,\alpha}^k; \quad \alpha \in \{x,y,z\}; \quad k = 1,\ldots,N, \quad (29b)$$

keeping in mind that the quantities $(v_0^k, \boldsymbol{V}_2^k) = (v_0^k, V_{2,x}^k, V_{2,y}^k, V_{2,z}^k)$ constitute the solution vector to the linear set of Eq. (24). These linear equations contain basic Gaussian integrals in the matrix (25) on the left-hand side, as well as integrals with the interaction terms of the Hamiltonian in the vector (28) on the right-hand side. The necessary integrals will be calculated analytically in Sec. III for condensates with rather general long-range interactions.

B. Dynamical equations for condensates with axial or spherical symmetry

If the GPE describes a system that is constrained by, for example, axial or spherical symmetry, the results obtained in

Sec. II A may be adapted to the case at hand. Therefore, we introduce respective coordinates (ϱ,ϕ,z) for axial symmetry and (r,θ,ϕ) for spherical symmetry and choose suitable trial wave functions,

$$\psi(\boldsymbol{r},t) = \sum_{k=1}^{N}\left[e^{i\gamma^k}\prod_{\alpha}\left(e^{ia_\alpha^k x_\alpha^2}\right)\right], \tag{30}$$

where for axially symmetric BEC we have $\alpha \in \{\varrho,z\}$, and for spherically symmetric, for example, monopolar BEC we have $\alpha = r$. These trial wave functions reduce the number of complex parameters to $3N$ $(a_\varrho^k,a_z^k,\gamma^k)$ and $2N$ (a_r^k,γ^k) $(k = 1,\ldots,N)$, respectively, where N is the number of Gaussians.

The procedure is the same as in Sec. II A: First, we calculate the time derivative $\dot{\psi}(t)$, which can be obtained by Eq. (16) by simply setting $a_x^k = a_y^k = a_\varrho^k$ and $a_x^k = a_y^k = a_z^k = a_r^k$, accordingly. Second, the Laplace operator is applied to the coupled Gaussian wave function, and, finally, with the respective definitions of the vectors $(v_0^k,1/2V_{2,\varrho}^k,1/2V_{2,z}^k)^{\mathrm{T}}$ and $(v_0^k,1/2V_{2,r}^k)^{\mathrm{T}}$, the dynamical equations can be written as

$$\begin{aligned}\dot{\gamma}^k &= 2i\left(2a_\varrho^k + a_z^k\right) - v_0^k,\\ \dot{a}_\alpha^k &= -4\left(a_\alpha^k\right)^2 - \tfrac{1}{2}V_{2,\alpha}^k; \quad k = 1,\ldots,N; \quad \alpha \in \{\varrho,z\}\end{aligned} \tag{31}$$

for a BEC with axial symmetry $(D = 2)$ and

$$\begin{aligned}\dot{\gamma}^k &= 6ia_r^k - v_0^k,\\ \dot{a}_r^k &= -4\left(a_r^k\right)^2 - \tfrac{1}{2}V_{2,r}^k; \quad k = 1,\ldots,N\end{aligned} \tag{32}$$

for a BEC with spherical symmetry $(D = 1)$. The quantities $(v_0^k,1/2V_{2,\varrho}^k,1/2V_{2,z}^k)^{\mathrm{T}}$ and $(v_0^k,1/2V_{2,r}^k)^{\mathrm{T}}$ have to be calculated from an adapted set of linear equations analogous to Eq. (23), but for a BEC with axial symmetry, $D = 2$, with

$$\alpha,\beta \in \{\varrho,z\}, \tag{33}$$

and for a BEC with spherical symmetry, $D = 1$, with

$$\alpha,\beta = r. \tag{34}$$

As in Eq. (24), we can rewrite both respective linear sets of equations in the form of a matrix equation,

$$\boldsymbol{M}\boldsymbol{v} = \boldsymbol{r}, \tag{35}$$

with the Hermitian, positive definite $(D+1)N \times (D+1)N$ matrix $\boldsymbol{M}$ analog to Eq. (25), but with a reduced number of blocks, $\{(\varrho^2)_{kl},(z^2)_{kl},\ldots\}$ or $\{(r^2)_{kl},\ldots\}$, and the $(D+1)$ N-dimensional respective vectors $\boldsymbol{v}$ and $\boldsymbol{r}$ for $D = 2$ and $D = 1$.

We have applied the TDVP of Dirac Frenkel and McLachlan to the extended GPE and a trial wave function with coupled Gaussian functions. With the resulting dynamical Eqs. (29), (31), and (32) in respective symmetries we can calculate the time dependence of the wave function ψ by calculating the time dependence of the variational parameters. To set up Eqs. (29), (31), and (32), we have to solve the set of linear equations for the quantities $(v_0^k,V_{2,\alpha}^k)$, $k = 1,\ldots,N$; $\alpha = x,y,z$ $(\alpha = \varrho,z$ and $\alpha = r$, respectively) in Eq. (23). All integrals of the matrix and the right-hand side are calculated analytically.

III. CALCULATION OF THE INTEGRALS

For clarity we sort all integrals as they appear in this matrix equation: the integrals for the matrix (25) in Sec. III A and the integrals of the right-hand side (28) in Sec. III B. Then we calculate the mean-field energy and the chemical potential for a BEC with long-range interaction in Sec. III C.

A. Computation of the matrix $\boldsymbol{M}$

The integrals of the matrix $\boldsymbol{M}$ in Eq. (25) are all of the form $\langle g^l \mid g^k\rangle$, $\langle g^l|x_\alpha^2|g^k\rangle$, and $\langle g^l|x_\alpha^2x_\beta^2|g^k\rangle$, with $x_\alpha,x_\beta \in \{x,y,z\}$, and each Gaussian function g^k defined in Eq. (13). All integrals are easily calculated from the simplest integral $\langle g^l \mid g^k\rangle$ with the use of the relation

$$\langle g^l|x_\alpha^{2\lambda}x_\beta^{2\nu}V|g^k\rangle = (-i)^{\lambda+\nu}\frac{\partial^\lambda}{\partial\left(a_\alpha^k\right)^\lambda}\frac{\partial^\nu}{\partial\left(a_\beta^k\right)^\nu}\langle g^l|V|g^k\rangle, \tag{36}$$

with $\lambda,\nu = 0,1,2,\ldots$, and V an arbitrary potential.

To facilitate reading and to shorten the extensive terms in integrals or integral solutions, we introduce the following abbreviations:

$$a_\alpha^{kl} = a_\alpha^k - \left(a_\alpha^l\right)^*, \tag{37a}$$
$$a_\alpha^{ij} = a_\alpha^i - \left(a_\alpha^j\right)^*, \tag{37b}$$
$$a_\alpha^{klij} = a_\alpha^{kl} + a_\alpha^{ij}, \quad \alpha \in \{x,y,z\}, \tag{37c}$$
$$\gamma^{kl} = \gamma^k - (\gamma^l)^*, \tag{37d}$$
$$\gamma^{ij} = \gamma^i - (\gamma^j)^*, \tag{37e}$$
$$\gamma^{klij} = \gamma^{kl} + \gamma^{ij}. \tag{37f}$$

We start with

$$\begin{aligned}\langle g^l \mid g^k\rangle &= e^{i\gamma^{kl}}\int_{-\infty}^{\infty}e^{ia_x^{kl}x^2}dx\int_{-\infty}^{\infty}e^{ia_y^{kl}y^2}dy\int_{-\infty}^{\infty}e^{ia_z^{kl}z^2}dz\\ &= \frac{\pi^{3/2}e^{i\gamma^{kl}}}{\sqrt{-ia_x^{kl}}\sqrt{-ia_y^{kl}}\sqrt{-ia_z^{kl}}},\end{aligned} \tag{38}$$

where, as can be seen easily from the definition of the Gaussian trial wave function (4), the imaginary parts of the widths are to remain positive. Therefore, the imaginary parts of the occurring combinations also fulfill $\mathrm{Im}[a^k - a^{l*}] > 0$.

The application of the relation (36) to the norm integral (38) provides with $\lambda = 1$, $\nu = 0$ the integrals

$$\langle g^l|x^2|g^k\rangle = \frac{\pi^{3/2}e^{i\gamma^{kl}}}{2\left(-ia_x^{kl}\right)^{3/2}\sqrt{-ia_y^{kl}}\sqrt{-ia_z^{kl}}}, \tag{39a}$$

$$\langle g^l|y^2|g^k\rangle = \frac{\pi^{3/2}e^{i\gamma^{kl}}}{2\sqrt{-ia_x^{kl}}\left(-ia_y^{kl}\right)^{3/2}\sqrt{-ia_z^{kl}}}, \tag{39b}$$

$$\langle g^l|z^2|g^k\rangle = \frac{\pi^{3/2}e^{i\gamma^{kl}}}{2\sqrt{-ia_x^{kl}}\sqrt{-ia_y^{kl}}\left(-ia_z^{kl}\right)^{3/2}}, \tag{39c}$$

and with $\lambda + \nu = 2$ the integrals

$$\langle g^l|x^4|g^k\rangle = \frac{3\pi^{3/2}e^{i\gamma^{kl}}}{4\left(-ia_x^{kl}\right)^{5/2}\sqrt{-ia_y^{kl}}\sqrt{-ia_z^{kl}}}, \tag{40a}$$

$$\langle g^l|y^4|g^k\rangle = \frac{3\pi^{3/2}e^{i\gamma^{kl}}}{4\sqrt{-ia_x^{kl}}\left(-ia_y^{kl}\right)^{5/2}\sqrt{-ia_z^{kl}}}, \tag{40b}$$

$$\langle g^l|z^4|g^k\rangle = \frac{3\pi^{3/2}e^{i\gamma^{kl}}}{4\sqrt{-ia_x^{kl}}\sqrt{-ia_y^{kl}}\left(-ia_z^{kl}\right)^{5/2}}, \tag{40c}$$

and

$$\langle g^l|x^2y^2|g^k\rangle = \frac{\pi^{3/2}e^{i\gamma^{kl}}}{4\left(-ia_x^{kl}\right)^{3/2}\left(-ia_y^{kl}\right)^{3/2}\sqrt{-ia_z^{kl}}}, \tag{41a}$$

$$\langle g^l|x^2z^2|g^k\rangle = \frac{\pi^{3/2}e^{i\gamma^{kl}}}{4\left(-ia_x^{kl}\right)^{3/2}\sqrt{-ia_y^{kl}}\left(-ia_z^{kl}\right)^{3/2}}, \tag{41b}$$

$$\langle g^l|y^2z^2|g^k\rangle = \frac{\pi^{3/2}e^{i\gamma^{kl}}}{4\sqrt{-ia_x^{kl}}\left(-ia_y^{kl}\right)^{3/2}\left(-ia_z^{kl}\right)^{3/2}}. \tag{41c}$$

Since the matrix is now complete, we turn to the more challenging integrals needed for the right-hand side of Eq. (24), that is, the vector $\boldsymbol{r}$ defined in Eq. (28).

B. Computation of the vector r

The right-hand side of Eq. (24) contains the trapping term, V_t, the scattering term, $V_{\rm sc}$, and the more complicated long-range interaction term, $V_{\rm lr}$. In the following equations, the g^k defined in Eq. (13) represents the individual Gaussians of the trial wave function.

1. Trapping

We start with the term of the trapping potential,

$$\begin{aligned}\langle g^l|V_t|g^k\rangle &= \langle g^l|\gamma_x^2x^2+\gamma_y^2y^2+\gamma_z^2z^2|g^k\rangle \\ &= \frac{\pi^{3/2}e^{i\gamma^{kl}}\left(\gamma_x^2a_y^{kl}a_z^{kl}+\gamma_y^2a_x^{kl}a_z^{kl}+\gamma_z^2a_x^{kl}a_y^{kl}\right)}{2\left(-ia_x^{kl}\right)^{3/2}\left(-ia_y^{kl}\right)^{3/2}\left(-ia_z^{kl}\right)^{3/2}}.\end{aligned} \tag{42}$$

For the right-hand side of Eq. (24) we also need the terms

$$\langle g^l|x_\alpha^2V_t|g^k\rangle,$$

with $x_\alpha \in \{x,y,z\}$. They are directly obtained with the help of Eqs. (40) and (41).

2. Scattering

The second interaction term of $V_{\rm eff}$ on the right-hand side of Eq. (24) contains the nonlinear contact interaction $V_{\rm sc} = 8\pi a_{\rm sc}|\psi(\boldsymbol{r})|^2$ of the s-wave scattering. Following the same procedure as earlier, we start by calculating $\langle g^l|V_{\rm sc}|g^k\rangle$, before obtaining the terms $\langle g^l|x_\alpha^2V_{\rm sc}|g^k\rangle$ with $x_\alpha \in \{x,y,z\}$ using the relation (36),

$$\begin{aligned}\langle g^l|V_{\rm sc}|g^k\rangle &= \langle g^l|8\pi a_{\rm sc}|\psi|^2|g^k\rangle \\ &= \sum_{i,j=1}^{N}\int d^3\boldsymbol{r}\left(8\pi a_{\rm sc}.g^l(\boldsymbol{r})^*g^j(\boldsymbol{r})^*g^k(\boldsymbol{r})g^i(\boldsymbol{r})\right) \\ &= 8a_{\rm sc}\pi^{5/2}\sum_{i,j=1}^{N}\frac{e^{i\gamma^{klij}}}{\sqrt{-ia_x^{klij}}\sqrt{-ia_y^{klij}}\sqrt{-ia_z^{klij}}},\end{aligned} \tag{43}$$

as long as $\mathrm{Im}\,a_\alpha^{klij} > 0$ for $\alpha \in \{x,y,z\}$, which is true [see Eq. (37) and note that $\mathrm{Im}[a_\alpha^k] > 0$ for all width parameters]. Again we use relation (36) and get the three remaining integrals:

$$\langle g^l|x^2V_{\rm sc}|g^k\rangle = 4a_{\rm sc}\pi^{5/2}\sum_{i,j=1}^{N}\frac{e^{i\gamma^{klij}}}{\left(-ia_x^{klij}\right)^{3/2}\sqrt{-ia_y^{klij}}\sqrt{-ia_z^{klij}}}, \tag{44a}$$

$$\langle g^l|y^2V_{\rm sc}|g^k\rangle = 4a_{\rm sc}\pi^{5/2}\sum_{i,j=1}^{N}\frac{e^{i\gamma^{klij}}}{\sqrt{-ia_x^{klij}}\left(-ia_y^{klij}\right)^{3/2}\sqrt{-ia_z^{klij}}}, \tag{44b}$$

$$\langle g^l|z^2V_{\rm sc}|g^k\rangle = 4a_{\rm sc}\pi^{5/2}\sum_{i,j=1}^{N}\frac{e^{i\gamma^{klij}}}{\sqrt{-ia_x^{klij}}\sqrt{-ia_y^{klij}}\left(-ia_z^{klij}\right)^{3/2}}. \tag{44c}$$

3. Long-range interaction

The most challenging calculation surely is that of the long-range interaction term $V_{\rm lr} = \int d^3\boldsymbol{r}'W_{\rm lr}(\boldsymbol{r}-\boldsymbol{r}')|\psi(\boldsymbol{r}')|^2$ [see Eq. (1)],

$$\begin{aligned}\langle g^l|V_{\rm lr}|g^k\rangle = \sum_{i,j=1}^{N}\int d^3\boldsymbol{r}\int d^3\boldsymbol{r}'W_{\rm lr}(\boldsymbol{r}-\boldsymbol{r}')g^{j*}(\boldsymbol{r}') \\ \times g^i(\boldsymbol{r}')g^{l*}(\boldsymbol{r})g^k(\boldsymbol{r}).\end{aligned} \tag{45}$$

Introducing relative (rel) and "center-of mass" (c.m.) coordinates via

$$\begin{pmatrix}\boldsymbol{r}\\ \boldsymbol{r}'\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}\begin{pmatrix}\boldsymbol{r}_{\rm rel}\\ \boldsymbol{r}_{\rm c.m.}\end{pmatrix}, \tag{46}$$

and keeping the Jacobian determinant (1/8) in mind, Eq. (45) is transformed to

$$\begin{aligned}\langle g^l|V_{\rm lr}|g^k\rangle = \sum_{i,j=1}^{N}\frac{e^{i\gamma^{klij}}}{8}\int d^3\boldsymbol{r}_{\rm rel}\int d^3\boldsymbol{r}_{\rm c.m.}W_{\rm lr}(\boldsymbol{r}_{\rm rel}) \\ \times\exp\Big\{\frac{i}{4}\big(a_x^{kl}(x_{\rm c.m.}+x_{\rm rel})^2+a_y^{kl}(y_{\rm c.m.}+y_{\rm rel})^2 \\ +a_z^{kl}(z_{\rm c.m.}+z_{\rm rel})^2+a_x^{ij}(x_{\rm c.m.}-x_{\rm rel})^2 \\ +a_y^{ij}(y_{\rm c.m.}-y_{\rm rel})^2+a_z^{ij}(z_{\rm c.m.}-z_{\rm rel})^2\big)\Big\},\end{aligned} \tag{47}$$

with the abbreviations (37). We use the integral

$$\int_{-\infty}^{\infty}e^{i[a(x+u)^2+b(x-u)^2]}dx = \frac{\sqrt{\pi}}{\sqrt{-i(a+b)}}e^{i\frac{4abu^2}{a+b}}, \tag{48}$$

which, for $\mathrm{Im}[a+b] > 0$, is easily transformed into a standard Gaussian integral after completing the square in the exponent, and solve the center-of-mass integral in Eq. (47)

$$\langle g^l|V_{\rm lr}|g^k\rangle = \sum_{i,j=1}^{N}\pi^{3/2}\frac{e^{i\gamma^{klij}}}{\sqrt{ia_x^{klij}a_y^{klij}a_z^{klij}}}I_{\rm rel}^{klij}, \tag{49}$$

with

$$I_{\mathrm{rel}}^{klij} = \int d^3\boldsymbol{r}_{\mathrm{rel}} \left[W_{\mathrm{lr}}(\boldsymbol{r}_{\mathrm{rel}}) \exp\left\{ i \left(\frac{a_x^{ij} a_x^{kl}}{a_x^{klij}} x_{\mathrm{rel}}^2 + \frac{a_y^{ij} a_y^{kl}}{a_y^{klij}} y_{\mathrm{rel}}^2 + \frac{a_z^{ij} a_z^{kl}}{a_z^{klij}} z_{\mathrm{rel}}^2 \right) \right\} \right]. \quad (50)$$

The relative integral I_{rel}^{klij} depends on the specific form of the two-particle interatomic interaction $W_{\mathrm{lr}}(\boldsymbol{r}_{\mathrm{rel}})$. The integral obtained with the coupled Gaussian method is formally the same as for the calculation with a single Gaussian trial wave function, except for the complex coefficients in the exponent, $a_\alpha^{ij} a_\alpha^{kl} / a_\alpha^{klij}$ for $\alpha \in \{x,y,z\}$. Therefore, the method of coupled Gaussian functions is applicable to all two-particle long-range interactions which can be solved with the simple single Gaussian wave function.

As an example, we present the results for the relative integral for dipolar interaction

$$W_{\mathrm{lr}}(\boldsymbol{r}_{\mathrm{rel}}) = W_d(\boldsymbol{r}_{\mathrm{rel}}) = \frac{1 - 3\frac{z_{\mathrm{rel}}^2}{|\boldsymbol{r}_{\mathrm{rel}}|^2}}{|\boldsymbol{r}_{\mathrm{rel}}|^3}, \quad (51)$$

where I_{rel} can be expressed in terms of elliptic integrals [16,17],

$$I_{\mathrm{rel}} = \frac{4\pi}{3}\left[\kappa_x \kappa_y R_D\left(\kappa_x^2, \kappa_y^2, 1\right) - 1\right]. \quad (52)$$

κ_x, κ_y are complex combinations of the Gaussian widths,

$$\kappa_x = \sqrt{\frac{a_x^{klij} a_z^{ij} a_z^{kl}}{a_x^{ij} a_x^{kl} a_z^{klij}}}, \quad \kappa_y = \sqrt{\frac{a_y^{klij} a_z^{ij} a_z^{kl}}{a_y^{ij} a_y^{kl} a_z^{klij}}},$$

and R_D is the elliptic integral of the second kind in Carlson form [22,23],

$$R_D(x,y,z) = \frac{3}{2}\int_0^\infty \frac{dt}{\sqrt{(x+t)(y+t)(z+t)^3}}.$$

Numerically it is convenient to use Carlson's formulation for elliptic integrals because there are very fast converging algorithms available [22,23] even for complex arguments $x,y,z \in \mathbb{C}$.

The three additional integrals $\langle g^l | x_\alpha^2 V_{\mathrm{lr}} | g^k \rangle$ for $x_\alpha \in \{x,y,z\}$ needed to complete Eq. (24) are obtained using derivatives of $\langle g^l | V_{\mathrm{lr}} | g^k \rangle$ with respect to the Gaussian widths a_α^k [see Eq. (36)],

$$\langle g^l | x_\alpha^2 V_{\mathrm{lr}} | g^k \rangle = -i \frac{\partial}{\partial a_\alpha^k} \langle g^l | V_{\mathrm{lr}} | g^k \rangle.$$

C. Energy functional and chemical potential

We calculate the mean-field energy and the chemical potential,

$$E_{\mathrm{mf}} = \sum_{k,l=1}^{N} \langle g^l | -\Delta + V_t + \tfrac{1}{2}(V_{\mathrm{sc}} + V_{\mathrm{lr}}) | g^k \rangle, \quad (53a)$$

$$\mu = \sum_{k,l=1}^{N} \langle g^l | -\Delta + V_t + V_{\mathrm{sc}} + V_{\mathrm{lr}} | g^k \rangle. \quad (53b)$$

The terms for trapping, scattering, and the long-range interaction are evaluated in Sec. III B. We now calculate the kinetic term and apply the Laplace operator to the coupled Gaussian wave function,

$$\langle g^l | \Delta | g^k \rangle = \frac{-2\pi^{3/2} e^{i\gamma^{kl}}}{\left(i a_x^{kl} a_y^{kl} a_z^{kl}\right)^{1/2}} \sum_{\alpha=x,y,z} \left\{ \frac{\left(a_\alpha^k\right)^2}{-i a_\alpha^{kl}} - i a_\alpha^k \right\}. \quad (54)$$

Now, all integrals that are needed for the linear equations for the quantities $(v_0^k, V_{2,\alpha}^k)$, $k = 1,\ldots,N; \alpha = x,y,z$ in Eq. (23), as well as all integrals for the mean-field energy and the chemical potential have been calculated. We are able to set up the dynamical equations for the Gaussian parameters. These dynamical equations can be solved using three different methods, either by minimization of the mean-field energy, by the search for fixed points of the dynamical equations, or by imaginary time evolution of an initial wave function.

IV. COMPUTATION OF THE GROUND STATE AND EXCITED STATES

There are three different methods available for calculating variational solutions. The solutions obtained via minimization of the mean-field energy or via evolution of an initial wave function in imaginary time, are limited to the stable ground state. The method of a highly nonlinear root search of the dynamical Eqs. (29) yields all stationary states of the GPE, the ground state, and collectively excited states.

The sensitivity of the methods on the initial values greatly differs. While the minimization and the imaginary time evolution are relatively robust, the root search requires sufficiently accurate parameters, especially for an increasing number of variational parameters. For more coupled Gaussian functions, however, the minimization of the mean-field energy and the imaginary time evolution get increasingly time consuming. Results should therefore be obtained with the nonlinear root search, the other two routines should only be used to calculate appropriate initial values.

A. Minimization of the mean-field energy

One method of obtaining the ground state of the GPE is to minimize the mean-field energy functional in Eq. (2). For multiple coupled Gaussians, the analytical calculation of all derivatives with respect to the variational parameters, for example, for calculating the gradient, is not possible. Therefore, we use a numerical minimization routine that uses the energy function values only. For an increased number of Gaussian parameters, the accuracy of this method is limited, but the results may be used as initial values for a root search of the dynamical equations, which provides much more reliable and accurate results.

B. Root search for fixed points of the dynamical equations

The full three-dimensional calculation for condensates with long-range interaction includes $4N$ complex variational parameters of the wave function. We search for these solutions

of the nonlinear dynamical Eqs. (29), (31), and (32) where the dynamic is trivial, that is, the stationary states. The phase of all Gaussians is defined by the chemical potential [see Eq. (55)].

We use a wave function with N complex amplitude and phase parameters $\gamma^k,\ldots,\gamma^N$. Since the wave function has to be normalized, we have to ensure $\langle\psi|\psi\rangle = 1$. In summary, we have to find roots of the following system of equations:

$$\begin{aligned}
\dot{a}_x^k &= -4\left(a_x^k\right)^2 - \tfrac{1}{2}V_{2,x}^k \stackrel{!}{=} 0,\\
\dot{a}_y^k &= -4\left(a_y^k\right)^2 - \tfrac{1}{2}V_{2,y}^k \stackrel{!}{=} 0,\\
\dot{a}_z^k &= -4\left(a_z^k\right)^2 - \tfrac{1}{2}V_{2,z}^k \stackrel{!}{=} 0,\\
\dot{\gamma}^k &= 2i\left(a_x^k + a_y^k + a_z^k\right) - v_0^k \stackrel{!}{=} -\mu,\\
\langle\psi \mid \psi\rangle &- 1 \stackrel{!}{=} 0,
\end{aligned} \tag{55}$$

for $k = 1,\ldots,N$. The quantities v_0 and $V_{2,x,y,z}$ constitute the solution vector to the set of Eqs. (23). The right-hand side (28) of this set of equations contains the integrals of contact, trap, and long-range interaction. The calculation of the dipolar interaction yields elliptic integrals which are evaluated with the help of fast converging algorithms [22,23].

The root search itself is highly nonlinear and may be performed with an algorithm based on the Powell hybrid method [24]. The success and the speed of any numerical root search greatly depends on the number of variational parameters. Therefore, we reduce the number of parameters prior to this routine as much as possible. Since the ground state of, for example, dipolar condensates in an axially symmetric trap is axially symmetric, $a_x^k = a_y^k \equiv a_\varrho^k$, it is possible to reduce the first $3N$ equations in Eqs. (55) to $2N$ equations. For condensates with $1/r$ interaction, the wave function as well as the stationary states are spherically symmetric. Therefore, we are able to further reduce the number of width parameters using $a_x^k = a_y^k = a_z^k \equiv a_r^k$.

C. Imaginary time evolution

The third method for finding solutions of the GPE is the imaginary time evolution of an initial wave function. Although the calculation for a distinct scattering length may take a long time, the routine is rather insensitive to the choice of the initial parameter values, even for a large number of variational parameters. Therefore, the imaginary time evolution is very useful in the context of the calculation of very accurate input values for the root search.

We substitute $t \to \tau = it$ in the GPE and calculate the (imaginary) time evolution of the dynamical equations. For the linear Schrödinger equation this leads to a damping of all states with a factor according to their respective energy eigenvalues $\exp(-E_n\tau)$. Sufficiently long integration with respect to the imaginary time coordinate and renormalizing yields the ground state of the Hamiltonian. The method can also be applied to the nonlinear GPE.

In a next step, we linearize the dynamical equations in the vicinity of the fixed points in order to analyze the stability and possible bifurcations. We can also calculate fluctuations $\delta\psi$ of the stationary wave function.

V. STABILITY PROPERTIES OF THE VARIATIONAL FIXED POINTS

The standard method for analyzing the stability of solutions of the GPE is to perturb the wave function of the solution and linearize the GPE, which leads to the Bogoliubov–de Gennes equations [3]. In this section, we make a different approach and apply methods of nonlinear dynamics to analyze the stability of the condensates.

The application of the TDVP to a wave function consisting of coupled Gaussian functions in Sec. II led to a set of dynamical equations. In Sec. IV we described methods for searching for stationary solutions of the Eqs. (55). Minimization of the mean-field energy, imaginary time evolution, or root search yield variational parameters z^{FP} for stationary solutions of the GPE, so-called "fixed points" (FPs). In the case of N coupled Gaussian functions these parameters are $3N$ complex widths, N for each a_x^k,a_x^k,a_z^k and N complex amplitude and phase parameters γ^k:

$$z^{\mathrm{FP}} = \left(\gamma^k,a_x^k,a_y^k,a_z^k\right)^{\mathrm{FP}};\quad k = 1,\ldots,N. \tag{56}$$

In the case of an axially or spherically symmetric BEC, the procedure that follows is the same, but with reduced sets of subscripts, (ϱ,z) or even (r) for the width parameters.

We will investigate the stability of these stationary solutions with the help of a perturbation of the parameters at the fixed point. If the parameter set for the stationary solution is indeed the minimum of the mean-field energy, we expect the solution to be stable. In this case small changes of the variational parameters will only result in a quasiperiodic oscillation confined to the vicinity of the original fixed point. By contrast, as we will see, if the stationary fixed point is a hyperbolic fixed point, small perturbations will lead to an exponential growth of the solution. For the following calculation of the stability matrix, it is irrelevant which method was used to obtain the parameters of the stationary solution in the first place.

To observe the time dependence of the perturbations, we use the dynamical equations for the Gaussian parameters (29). The fixed point obviously fulfills Eqs. (55),

$$\begin{aligned}
\dot{\gamma}^k(z^{\mathrm{FP}}) &= -\mu,\\
\dot{a}_\alpha^k(z^{\mathrm{FP}}) &= 0,
\end{aligned} \tag{57}$$

for $\alpha = x,y,z$; $k = 1,\ldots,N$. For small deviations from the fixed point, we first split the preceding equations into real (Re) and imaginary (Im) parts (indicated with the tilde $z \to \tilde{z}$) in order to linearize them,

$$\delta\dot{\tilde{z}} = \boldsymbol{J}\delta\tilde{z}. \tag{58}$$

$\delta\tilde{z}$ denotes the deviation of the variational parameters from those at the fixed point, $\tilde{z} = \tilde{z}^{\mathrm{FP}} + \delta\tilde{z}$, and $\boldsymbol{J}$ denotes the

$8N \times 8N$-dimensional real valued Jacobian matrix at the fixed point

$$\boldsymbol{J} = \frac{\partial\left(\gamma^{k,\mathrm{Re}},\gamma^{k,\mathrm{Im}},a_\alpha^{k,\mathrm{Re}},a_\alpha^{k,\mathrm{Im}}\right)}{\partial\left(\gamma^{l,\mathrm{Re}},\gamma^{l,\mathrm{Im}},a_\beta^{l,\mathrm{Re}},a_\beta^{l,\mathrm{Im}}\right)}, \tag{59}$$

with $\alpha,\beta = x,y,z$ and $k,l = 1,\ldots,N$. The eigenvalues of $\boldsymbol{J}$ determine the characteristic stability of the fixed point in whose surroundings the linearization takes place. In the coordinates given by the eigenvectors of $\boldsymbol{J}$, all differential equations take the form

$$\delta\dot{\tilde{z}}_i = \lambda_i \delta\tilde{z}_i; \quad i = 1,\ldots,8N, \tag{60}$$

which have the simple solution

$$\delta\tilde{z}_i(t) = \delta\tilde{z}_i^0 e^{\lambda_i t}. \tag{61}$$

The eigenvalues occur in pairs; that is, if λ_i is an eigenvalue, $-\lambda_i$ is also an eigenvalue of $\boldsymbol{J}$. Since the Jacobian matrix is not symmetric, the eigenvalues λ_i are real or complex, and there are two possibilities. If all eigenvalues λ_i are purely imaginary, the time evolution of the perturbation remains confined, since the solution (61) is oscillating. In contrast, if at least one of the real parts of the eigenvalues ($\mathrm{Re}\,\lambda_i$) is nonzero, any perturbation in the direction of the corresponding eigenvector will grow exponentially.

Using this method we observe the behavior under small perturbations. We are able to investigate the stability of any fixed point that we obtain, for example, from a root search of the dynamical equations.

For unstable fixed points the methods of nonlinear dynamics also allow us to gain insight in the collapse mechanism by analyzing variations of the wave function characterized by the respective eigenvectors

$$\delta\tilde{z}_i = \left(\delta\gamma_i^{k,\mathrm{Re}},\delta\gamma_i^{k,\mathrm{Im}},\delta a_{\alpha,i}^{k,\mathrm{Re}},\delta a_{\alpha,i}^{k,\mathrm{Im}}\right)^{\mathrm{T}}, \tag{62}$$

with $k = 1,\ldots,N$; $\alpha \in \{x,y,z\}$. If this eigenvector $\delta\tilde{z}_i$ is axially symmetric, that is, $\delta a_{x,i}^k = \delta a_{y,i}^k$ for all k, the perturbation of the condensate is symmetric. If, however, the eigenvector breaks the axial symmetry, that is, $\delta a_{x,i}^k = -\delta a_{y,i}^k$ for all k, the perturbation leads to an asymmetric oscillation or collapse of the condensate, depending on whether the respective eigenvalue is purely real or imaginary.

With the variations of the variational parameters of the eigenvector we calculate the expansion of the wave function at the fixed point and get the solution for the linearized variation of the wave function

$$\delta\psi_i(\boldsymbol{r},t) = \sum_{k=1}^{N}\left(\sum_\alpha\left[i x_\alpha^2 \delta a_{\alpha,i}^{k,\mathrm{Re}} - x_\alpha^2 \delta a_{\alpha,i}^{k,\mathrm{Im}}\right] + i\delta\gamma_i^{k,\mathrm{Re}} - \delta\gamma_i^{k,\mathrm{Im}}\right) g^k|^{\mathrm{FP}}(\boldsymbol{r}) e^{\lambda_i t}, \tag{63}$$

with $\alpha \in \{x,y,z\}$. The respective eigenvalue is denoted λ_i and $g^k|^{\mathrm{FP}}$ is the unperturbed Gaussian k at the fixed point.

Is the approach based on the stability eigenvalues of the Jacobian fully equivalent to solutions of the Bogoliubov–de Gennes equations [3]? Probably not. Although the ansatz in Eq. (4) is quite general and not restricted to spherical or axial symmetric condensates, it allows for the description of the subset of excitations which are consistent with the ansatz (4). To obtain all solutions of the Bogoliubov–de Gennes equations with a variational approach, the ansatz must be further generalized. This will be the objective of future work.

VI. CONCLUSION

We used an ansatz with several coupled Gaussian functions to obtain an improved variational description of the dynamics of BECs. We applied a TDVP to the GPE and obtained dynamical equations for the variational parameters with the improved variational method of coupled Gaussian functions. We discussed methods for solving these equations and analyzing the stability using methods of nonlinear dynamics. When can we expect the proposed variational methods to be better than a grid method? This is hard to say in general. The variational ansatz with a finite number of Gaussians is still an approximation. However, grid calculations are only "exact" in the limit of a small step size and thus an infinitely large grid.

For a GPE with long-range monopolar ($1/r$) and dipolar ($1/r^3$) interaction, the improved variational results, the convergence, and comparisons with numerical calculations will be subject of the subsequent article [19]. It will be shown that a low number of Gaussians is sufficient to obtain converged results, and thus the number of parameters in the variational computations is significantly smaller compared to calculations on grids, and that a wealth of new phenomena is obtained by using the ansatz with coupled Gaussian functions.

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