Bose-Einstein condensates with attractive 1/*r* interaction: The case of self-trapping

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Amplifying on a proposal by O'Dell *et al.* for the realization of Bose-Einstein condensates of neutral atoms with attractive 1/*r* interaction, we point out that the instance of self-trapping of the condensate, without an external trap potential, is physically best understood by introducing appropriate "atomic" units. This reveals a remarkable scaling property: the physics of the condensate depends only on the two parameters $N^2 a/a_u$ and γ/N^2, where N is the particle number, a the scattering length, a_u the "Bohr" radius, and γ the trap frequency in atomic units. We calculate accurate numerical results for self-trapping wave functions and potentials, and for energies, sizes, and peak densities, and compare with previous variational results. We point out the existence of a second solution of the extended Gross-Pitaevskii equation for negative scattering lengths, with and without trapping potential, which is born together with the ground state in a tangent bifurcation. This indicates the existence of an unstable collectively excited state of the condensate for negative scattering lengths.

I. INTRODUCTION

Bose-Einstein condensation of *dipolar* gases has attracted much attention in recent years [1–5] because it offers the opportunity to create degenerate quantum gases with adjustable long- and short-range interactions, which gives rise to a wealth of novel phenomena [6–9]. In particular, the achievement of Bose-Einstein condensation in a gas of chromium atoms [10], with a large dipole moment, has opened the way to promising experiments on dipolar quantum gases [11].

As an alternative system with tunable interactions, the Bose-Einstein condensation of neutral atoms with electromagnetically induced attractive 1/*r* interaction has been proposed. Here a *monopolar*, "gravitylike," long-range interaction, in addition to the short-range (van der Waals–like) interactions, takes the place of the dipole-dipole interaction in dipolar gases. A monopolar quantum gas could be realized according to O'Dell *et al.* [12] by a combination of six appropriately arranged "triads" of intense off-resonant laser beams. In that arrangement, the $1/r^3$ interactions of the retarded dipole-dipole interaction of neutral atoms in the presence of intense electromagnetic radiation are averaged out in the near-zone limit [13,14], while the weaker 1/*r* interaction is retained. The resulting atom-atom interaction potential in the near-zone limit is [12]

$$V_u(\vec{r},\vec{r}') = -\frac{u}{|\vec{r}-\vec{r}'|}, \quad \text{with} \quad u = \frac{11}{4\pi}\frac{Ik^2\alpha^2}{c\varepsilon_0^2}.$$

Here, $\alpha(k)$ is the isotropic, dynamic, polarizability of the atoms at frequency ck and I the intensity of the radiation. The quantity u determines the strength of the "gravitylike" interaction. The estimate for u given by O'Dell *et al.* [12] for a CO_2 laser light of intensity $I=10^8$ W/cm² is equivalent to the attraction of two opposite equal charges with $q \approx e/2000$. However, by contrast with the van der Waals interaction, the 1/*r* potential acts over the entire sample, and

therefore its contribution to the energy can become important. Instead of six triads of lasers, a different arrangement with three rotating lasers has been proposed [15].

Even though the experimental realization of such configurations is not yet at hand, the theoretical issues associated with monopolar degenerate quantum gases are worthwhile investigating. In particular, as pointed out by O'Dell *et al.* [12], the intriguing new physical feature that emerges is the possibility of *self-trapping* of the condensate, without an external trap.

In the theory of trapped Bose-Einstein condensates it is common to introduce as natural units for energy and length the quantum energy $\hbar\omega_0$ and the oscillator length $a_0 = \sqrt{\hbar/m\omega_0}$ of the trap potential. In the case of self-trapping, however, where the trapping potential is switched off, $\hbar\omega_0 \to 0$ and $a_0 \to \infty$. Thus these quantities become "bad" units. As a consequence, in their study of the physical conditions necessary to observe the transition from external binding to self-binding Giovanazzi *et al.* [16] used the laser wavelength and energy as units of length and energy.

It is the purpose of this paper to reanalyze Bose condensates with attractive 1/*r* interaction using appropriate "atomic" units. This will first reveal remarkable scaling properties of the condensates. Next we solve the extended Gross-Pitaevskii equation for monopolar quantum gases numerically and compare with previous variational results. Last, we point out that our numerical calculations reveal the existence of a second solution of the Gross-Pitaevskii equation for negative scattering lengths, which is born together with the ground state in a bifurcation "out of nowhere." The existence of the second solution indicates the existence of an unstable collectively excited state of such condensates at negative scattering lengths.

II. NATURAL UNITS, SCALING PROPERTIES

A. General case

We analyze the physics of trapped monopolar gases, and in particular the limit $\omega_0 \to 0$, in terms of natural "atomic"

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units. From the analogy $u \Leftrightarrow e^2/4\pi\varepsilon_0$ we can define a "fine-structure constant"

$$\alpha_u := u/\hbar c \tag{1}$$

and can construct a "Bohr radius" and "Rydberg energy" in the usual way from the Compton wavelength $\lambdabar_C = \hbar/mc$ and the rest energy mc^2 via

$$a_u = \frac{\lambdabar_C}{\alpha_u} = \frac{\hbar^2}{mu}, \quad E_u = \frac{\alpha_u^2 mc^2}{2} = \frac{\hbar^2}{2ma_u^2}. \tag{2}$$

Measuring lengths in a_u and energies in E_u, we can write the Hartree equation of the ground state of a system of N identical bosons in an isotropic external trapping potential $V_0(r) = m\omega_0^2 r^2/2$, all in the same single-particle orbital ψ, interacting via V_u and the s-wave scattering pseudopotential $V_s = 4\pi a\hbar^2 \delta(\vec{r} - \vec{r}')/m$ in dimensionless form

$$\left[-\Delta + \gamma^2 r^2 + N 8\pi\frac{a}{a_u}|\psi(\vec{r})|^2 - 2N \int \frac{|\psi(\vec{r}')|^2}{|\vec{r} - \vec{r}'|} d^3\vec{r}' \right] \psi(\vec{r})$$
$$= \varepsilon\psi(\vec{r}). \tag{3}$$

In Eq. (3), ε is the chemical potential and the dimensionless quantity γ denotes the quantum energy of the trapping frequency in units of the "Rydberg" energy

$$\gamma = \hbar\omega_0/E_u. \tag{4}$$

Small values of γ imply that the effects of the trapping potential are small compared with the effects of the gravitylike interaction and vice versa for large values of γ. In Eq. (3) we have also assumed $N \gg 1$ so that the usual prefactor $(N-1)$ in the Hartree potential can be replaced with the total particle number N. Using the "order parameter" $\Psi = \sqrt{N}\psi$ instead of the single-particle orbital, one can absorb the N dependence in Eq. (3) in the wave function Ψ and obtain an extended (or, for vanishing gravitylike interaction, the familiar) time-independent Gross-Pitaevksii equation.

From Eq. (3) it would seem that there are three physical parameters governing the problem: the trap frequency ω_0, given by the dimensionless quantity γ, the particle number N, and the relative strength a/a_u of the scattering and the gravitylike potential. For the example mentioned before one has an estimate of $a \sim 10^{-9}$ m, $a_u \sim 2.5 \times 10^{-4}$, and thus $a/a_u \sim 10^{-6} - 10^{-5}$.

However, a central result of the present paper is that the physics of degenerate monopolar gases depends only on *two* relevant parameters: viz., γ/N^2 and $N^2 a/a_u$. To see this we note a remarkable scaling property of the mean-field Hamiltonian in Eq. (3): Let $\psi(\vec{r})$ be a solution of the (formal) *one*-boson problem for a given scaling length a/a_u and trap frequency γ,

$$H_{\mathrm{mf}}(N = 1, a/a_u, \gamma)(\vec{r})\psi(\vec{r}) = \varepsilon\psi(\vec{r}); \tag{5}$$

then, $\widetilde{\psi} := N^{3/2}\psi(\vec{\tilde{r}})$, with $\vec{\tilde{r}} = \vec{r}/N$, solves the N-boson problem for the scaled scattering length $N^2 a/a_u$ and the scaled trap frequency γ/N^2:
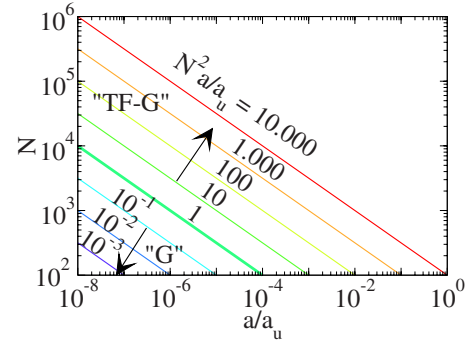

FIG. 1. (Color online) Phase diagram N vs a/a_u for the self-binding ground state of monopolar degenerate quantum gases (for the explanation, see text).

$$H_{\mathrm{mf}}(N, N^2 a/a_u, \gamma/N^2)(\vec{\tilde{r}})\widetilde{\psi}(\vec{\tilde{r}}) = \widetilde{\varepsilon}\widetilde{\psi}(\vec{\tilde{r}}), \tag{6}$$

with

$$\widetilde{\varepsilon} = N^2\varepsilon.$$

The proof is straightforward and left to the reader. From Eq. (6) follow scaling properties for the mean-field energy and the root-mean-square radius of the condensate and its peak density, respectively:

$$E(N, N^2 a/a_u, \gamma/N^2) = N^3 E(N = 1, a/a_u, \gamma),$$

$$\sqrt{\langle r^2 \rangle}|_{(N, N^2 a/a_u, \gamma/N^2)} = \sqrt{\langle r^2 \rangle}|_{(N=1, a/a_u, \gamma)}/\sqrt{N},$$

$$\varrho|_{(N, N^2 a/a_u, \gamma/N^2)} = N^4 \varrho|_{(N=1, a/a_u, \gamma)} = N^4|\psi(0)|^2. \tag{7}$$

Isosurfaces with constant $N^2 a/a_u$ and γ/N^2 form planes in the three-dimensional parameter space $(\gamma, N, a/a_u)$ on a logarithmic scale.

B. Self-binding

In the case of self-binding we are left with one relevant parameter, viz., $N^2 a/a_u$. In Fig. 1 we show the phase diagram N vs a/a_u for self-binding degenerate monopolar quantum gases. Note that because of the scaling property, the physics is identical on each of the sloping straight lines with $N^2 a/a_u = $const. Apart from a numerical factor, the relevant parameter $N^2 a/a_u$ is identical to the quantity $\widetilde{su}$ used by O'Dell *et al.* [12], but the universal nature of this quantity was not emphasized. The two asymptotic regimes of self-trapping dubbed "G" ("gravity") and "TF-G" ("Thomas-Fermi gravity") in Ref. [12] are characterized by the size of the scaling parameter. For $N^2 a/a_u \gg 1$, the kinetic energy is negligible and self-binding results from the balance between repulsive scattering and gravitylike attraction. For $N^2 a/a_u \ll 1$ scattering is negligible and self-trapping appears by a balance between kinetic energy and gravitylike attraction.

We note that the G regime corresponds to the Newton-Schrödinger scheme of quantum mechanics, which is a nonlinear variant of quantum mechanics that has been investi-
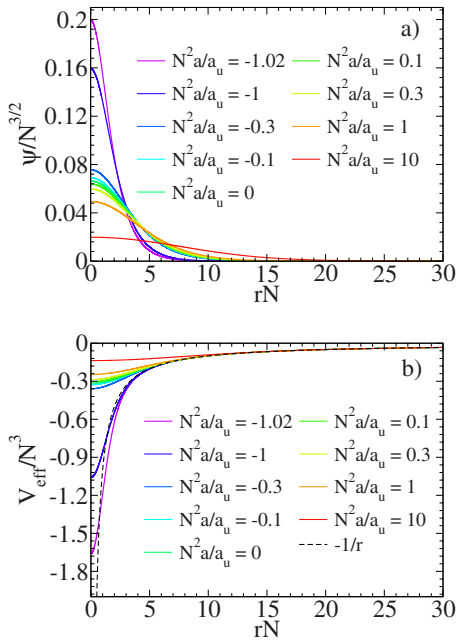
FIG. 2. (Color online) Numerically accurate self-binding ground-state s-wave solutions for different values of the scaling parameter N^2a/a_u: (a) wave functions and (b) self-binding potentials. Both in (a) the value of the wave function at the origin and in (b) the absolute value of the self-binding potential at the origin decrease monotonically with the scaling parameter from their maximum values at $N^2a/a_u=-1.02$ to their smallest values at $N^2a/a_u=10$. Thus, as the scaling parameter grows the binding becomes weaker. In (b) the asymptotic $1/r$ potential is also shown for comparison.

gated in detail in numerous publications on quantum measurement [17–24]. In that regime, the extended time-independent Gross-Pitaevskii equation (3) turns into the Schrödinger equation of gravitationally self-interacting quantum particles. It is worth noting that interacting monopolar quantum gases offer an experimental realization of Newton-Schrödinger quantum mechanics.

III. NUMERICAL SOLUTION, RESULTS, AND DISCUSSION

We have determined numerically accurate radially symmetric solutions of the extended Gross-Pitaevskii equation (3) in dependence on the scaling parameter N^2a/a_u both for the self-binding case $\gamma/N^2=0$ and for $\gamma/N^2\neq0$. To verify the numerical results two different methods were employed. One was to integrate in parallel Eq. (3) and the Poisson equation for the gravitylike interaction numerically outward from $r=0$ by exploiting the initial conditions for the first derivatives and setting initial values at $r=0$ for the wave function ψ_0 and the effective potential produced by the gravitylike interaction V_0. The latter was varied via bisection until convergence of the wave function to zero at large values of r was attained. The other method was an iterative one: the wave functions determined in the preceding step are used to calculate the effective potential in the next step, and the re-
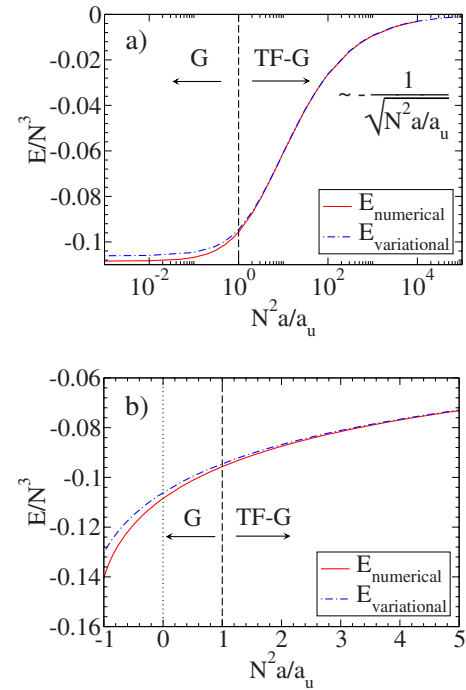

FIG. 3. (Color online) Total energy of the condensate as a function of N^2a/a_u: (a) on a logarithmic and (b) on a linear scale. Variational results obtained by minimizing the total energy for a Gaussian-type orbital [12] are shown by dashed lines.

sulting one-dimensional Schrödinger equation is integrated until self-consistency is achieved. The iteration is initialized by a reasonable guess for the wave function.

In Fig. 2 we show our results for the wave functions and the corresponding self-consistent potentials for the case of self-binding for different values of the scaling parameter N^2a/a_u. It can be seen that for increasing N^2a/a_u the potentials grow shallower and the wave functions become more extended. The figure confirms that asymptotically all self-binding potentials converge to a $1/r$ potential [24]. The case of $N^2a/a_u=0$ corresponds to solutions of the Newton-Schrödinger equation [24–27]. As already pointed out by O'Dell *et al.* [12], solutions also exist for negative scattering lengths, where the contact interaction, in addition to the gravitylike interaction, becomes attractive and stability of the condensate is established by the equilibrium of the kinetic energy of the condensate and the two attractive interactions. Figure 2 shows that for negative scattering lengths the self-trapping potentials become ever more binding, until at a value of $N^2a/a_u\approx-1.0251$ no solutions can be found anymore and the condensate becomes unstable with respect to collapse. This corrects the variational value of $N^2a/a_u=-3\pi/8\approx-1.18$ given by O'Dell *et al.* [12]. In their variational calculation, a Gaussian-type orbital was assumed and the mean-field energy of the condensate was minimized with respect to the width of the Gaussian.

Since we have the numerically accurate solutions at hand, we are in a position to check the accuracy of the variational results for observables of the condensate obtained by O'Dell *et al.* [12]. Figure 3 shows the behavior of the total energy of the condensate over seven decades of the scaling parameter
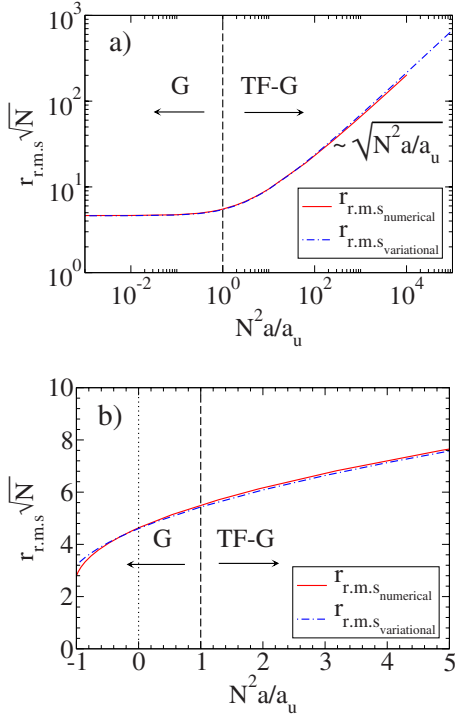
FIG. 4. (Color online) Root-mean-square radius of the condensate as a function of N^2a/a_u: (a) on a logarithmic and (b) on a linear scale. Variational results [12] are shown by dashed lines.

N^2a/a_u. To cover the range of negative scattering lengths, the energy is also given on a linear scale in the range around $N^2a/a_u \approx 0$. The transition between the two asymptotic regimes G and TF-G around $N^2a/a_u \sim 1$ is evident from Fig. 3. The comparison with the variational results also plotted in Fig. 3 shows that the TF-G regime is well described by the variational calculation. It is only in the transition to the G regime, and in particular for negative values of N^2a/a_u, that sizable deviations can be observed, up to the order of 10%.

Observables other than the energy are more sensitive to the accuracy of the wave function. We therefore compare our numerically accurate results with the variational results for the root-mean-square radius and the peak density of the condensate in Figs. 4 and 5, again over seven decades of the scaling parameter on a logarithmic scale and on a linear scale around $N^2a/a_u \approx 0$. Again, the transition between the two asymptotic regimes can be seen. It can also be recognized that the variational results well reproduce the overall behavior of the observables. For the extension of the condensate sizable deviations occur again in the transition to the G regime and for negative values of N^2a/a_u, while for the peak density the variational calculation overestimates the correct values in the TF-G regime and underestimates them in the G regime and for negative scattering lengths. Here the deviations increase up to more than 100%. This is understandable since the peak density depends crucially on the correct wave function.

IV. BIFURCATING SOLUTIONS

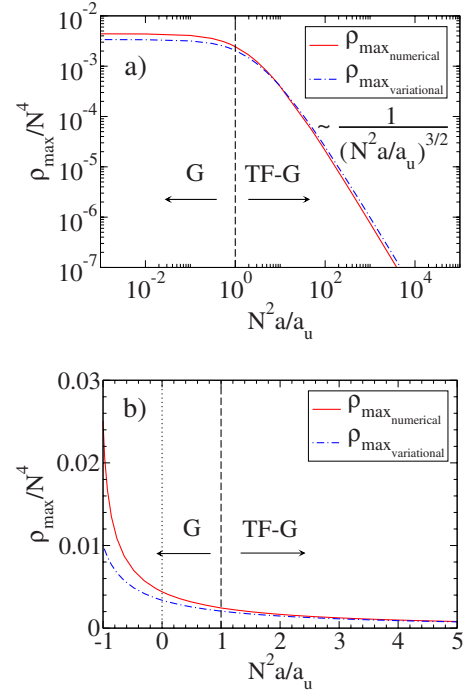A new result of our numerical calculations is that for negative scattering lengths there exists a second radially

FIG. 5. (Color online) Peak density ϱ of the condensate as a function of N^2a/a_u: (a) on a logarithmic and (b) on a linear scale. Variational results [12] are shown by dashed lines.

symmetric nodeless solution of the extended Gross-Pitaevskii equation (3). In Fig. 6 the chemical potentials of the two solutions are plotted as functions of the scaling parameter N^2a/a_u for $\gamma=0$. It is evident that the critical value
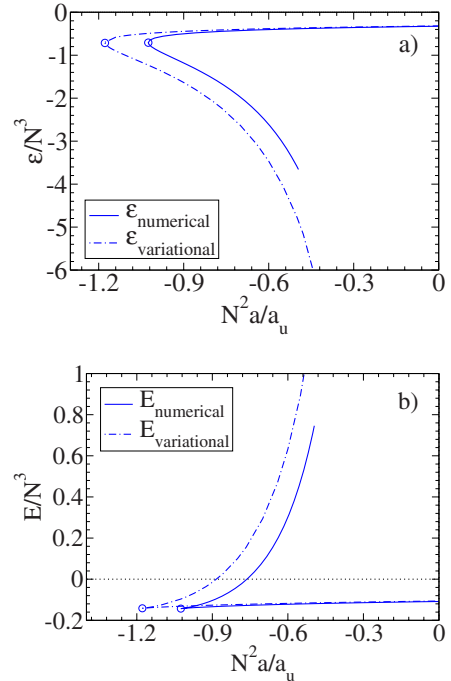

FIG. 6. (Color online) (a) Bifurcation of the chemical potential and (b) bifurcation of the total mean-field energy at the critical point $N^2a/a_u=-1.0251$, for self-binding—i.e., vanishing trap potential.
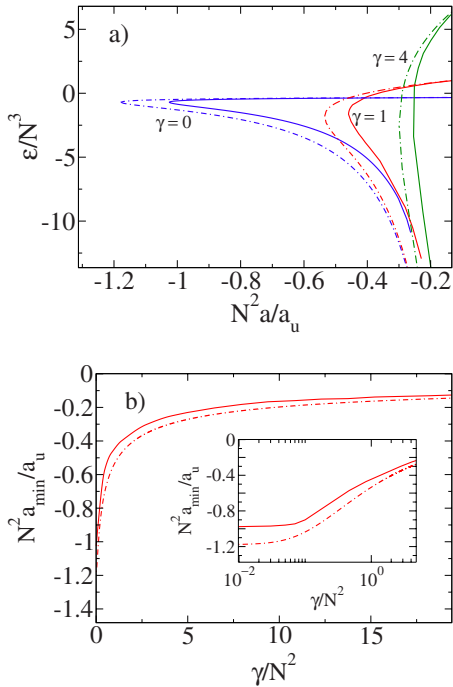
FIG. 7. (Color online) (a) Bifurcations of the chemical potential for nonvanishing values of the trapping potential. The case $\gamma=0$ is shown for comparison. (b) Dependence of the critical scattering length (the bifurcation point) on the frequency of the trapping potential. Numerically accurate results are given by solid lines, variational results by dashed lines. To elucidate the behavior for small values of γ/N^2, this region is shown in the inset on a logarithmic scale.

of $N^2a/a_u=-1.0251$ corresponds to a bifurcation point of the eigenvalue spectrum of Eq. (3): below the critical point no solution exists; at the critical point two solutions appear in a tangent bifurcation. The total energies of the condensates corresponding to the two solutions are also shown in Fig. 6. It can be seen that the energy increases from the bifurcation point on for the second solution. This would mean that above the bifurcation point there exists a *collective excited state* of the condensate in which all atoms occupy one and the same nodeless orbital, just like in the true ground state.

The second solution is in fact present also in the variational calculation. It there appears as a second stationary (maximum) point of the mean-field energy given as a function of the width of the Gaussian-type orbital. The variational results for the chemical potential and the total energy of the second solution are also included in Fig. 6. It can be seen that a numerically accurate calculation is necessary for a quantitative description of the bifurcation.

The second solution even persists in external trapping potentials for any value of γ. The bifurcation diagram for two finite values of γ is shown in Fig. 7. It can be seen that with growing γ the bifurcation point is shifted to smaller absolute values of N^2a/a_u. The increase of the total energy of the second solution which is evident from the figures is a consequence of the fact that the self-consistent potentials become more and more binding and the wave functions more and more localized, which leads to a dramatic increase in the kinetic energy.

What is the physical meaning of the second solution?

We note, on the one hand, that it corresponds to a maximum of the mean-field energy functional. Schrödinger's equation, however, and in our case Eq. (3), follows as the Euler-Lagrange equation of a variational principle which only demands the energy functional to be an extremum. Thus the fact that the second solution corresponds to a maximum of the energy functional does not preclude it from corresponding to a real physical quantum state. On the other hand, the two solutions are nodeless and hence nonorthogonal. Obviously, this is a consequence of the nonlinearity of the extended Gross-Pitaevskii equation (3): each solution creates its own self-consistent potential and thus sees a different Hamiltonian. This would seem surprising since the original many-body Hamiltonian is Hermitian and linear in the wave function, and therefore should possess only orthogonal eigenstates. The nonlinearity of Eq. (3) is a result of the Hartree approximation made for the states.

In studies of the decay rates in attractive trapped Bose-Einstein condensates, with contact interaction only, Huepe *et al.* [28,29] have seen similar behavior; i.e., a second solution is born in a tangent bifurcation together with the ground state. These states also are nonorthogonal. Analyzing the stability of the states, Huepe *et al.* have shown that the first excited state out of the two solutions is unstable with respect to macroscopic quantum tunneling.

This is a strong indication that the second solution found in this paper in Bose condensates with gravitylike interaction also corresponds to an unstable collectively excited state. A way to establish this is to linearize the time-dependent Gross-Pitaevskii equation corresponding to (3) around the stationary states and to carry out a stability analysis, as was done for the case of a pure attractive contact interaction by Huepe *et al.* [28,29]. Alternatively, by choosing a Gaussian ansatz with time-dependent widths [30], equations of motion for the widths can be obtained from the time-dependent Gross-Pitaevskii equation and analyzed with standard stability methods of nonlinear dynamics. Investigations along these lines are under way.

We finally note that there is an analogy with bifurcations seen in investigations of attractive one-dimensional Bose-Einstein condensates on a ring (cf., e.g., [31–33]). There, at a critical value of the ratio of the mean-field interaction energy to the kinetic energy, symmetry-breaking, solitonlike solutions appear, in addition to the symmetry-preserving solution of the Gross-Pitaevskii equation, which are lower in energy. By contrast, in the example discussed in this paper, both bifurcating solutions possess the same symmetry.

V. CONCLUSIONS

We have reanalyzed Bose condensates with attractive $1/r$ interaction by introducing appropriate atomic units which are in particular adapted to the case of self-binding. We have thus been able to derive previously unknown scaling properties of such condensates. We have calculated numerically accurate results for wave functions and observables of self-binding condensates and compared them with previous variational results. It turned out that in particular at negative scat-

tering lengths the variational results become poor and have to be replaced with our accurate numerical results. We have demonstrated that the critical point where collapse of the condensate occurs at negative scattering lengths is in reality a bifurcation point of the energy functional where both the ground state and an excited state merge and disappear. We have argued that this second solution indicates the existence of an unstable collectively excited state at negative scattering lengths in degenerate Bose condensates with long-range attractive $1/r$ interaction.

Critical points, below which collapse of the condensate sets in, not only exist in attractive condensates at negative scattering lengths [28–33] and in the monopolar gases with gravitylike interaction discussed in this paper, but also exist in dipolar gases, in certain parameter ranges of the particle number, the scattering length, and the trap frequencies [1,34,35]. Our investigations suggest that these also correspond to bifurcation points. Studies of the bifurcation scenarios in dipolar gases are therefore strongly encouraged.

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