Thomas-Fermi Approximation for a Condensate with Higher-order Interactions

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We consider the ground state of a harmonically trapped Bose-Einstein condensate within the Gross-Pitaevskii theory including the effective-range corrections for a two-body zero-range potential. The resulting non-linear Schrödinger equation is solved analytically in the Thomas-Fermi approximation neglecting the kinetic energy term. We present results for the chemical potential and the condensate profiles, discuss boundary conditions, and compare to the usual Thomas-Fermi approach. We discuss several ways to increase the influence of effective-range corrections in experiment with magnetically tunable interactions. The level of tuning required could be inside experimental reach in the near future.

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I. INTRODUCTION

The Gross-Pitaevskii (GP) equation \[ \hat{H} \Psi = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) + U_0 \left( |\Psi|^2 + g_2 \nabla^2 |\Psi|^2 \right) \right] \Psi, \tag{1} \]

where \( m \) is the atomic mass, \( V(r) \) is the external trap, \( U_0 = 4\pi\hbar^2 a/m \), and \( g_2 = a^2/3 - ar_e/2 \), with \( a \) and \( r_e \) being, respectively, the s-wave scattering length and effective range. We assume an isotropic trap, \( V(r) = m\omega^2 r^2/2 \), and introduce the trap length \( b = \sqrt{\hbar/m\omega} \). The single-particle density, \( \rho(r) = |\Psi(r)|^2 \), is normalized to the particle number, \( N = \int dr \rho(r), \) and \( \mu \) is the chemical potential.

As the boundary conditions are important for the TF approximation applied below we now discuss the procedure for obtaining the modified GP equation from the corresponding energy functional which is

\[ E(\Psi) = \int dr (\epsilon_K + \epsilon_V + \epsilon_I + \epsilon_{I2}), \tag{2} \]
with kinetic, potential, and interaction energy densities
\[ \epsilon_K = \frac{\hbar^2}{2m} |\nabla \Psi|^2, \quad \epsilon_V = V(r)|\Psi|^2, \quad \epsilon_I = \frac{1}{4} U_0 |\Psi|^4, \quad \epsilon_{I2} = \frac{1}{2} U_0 g_2 |\Psi|^2 \nabla^2 |\Psi|^2. \]
(3)

The corresponding integrated energy contributions are denoted \( E_K, E_V, E_I, \) and \( E_{I2} \), respectively. To obtain Eq. (1), we vary Eq. (2) with respect to \( \Psi^* \) for fixed \( \Psi \). To first order in \( \delta \Psi^* \), we have
\[ \delta E = E[\Psi^* + \delta \Psi^*] - E[\Psi^*] = \int dr \left[ - \frac{\hbar^2}{2m} \nabla^2 \Psi + V(r) \Psi + U_0 \left(|\Psi|^2 + g_2 \nabla^2 |\Psi|^2\right) \Psi \right] \delta \Psi^* \]
(4)
\[ + \int dS \cdot |\Psi|^2 \nabla (\Psi \delta \Psi^*) - \int dS \cdot \Psi \delta \Psi^* \nabla |\Psi|^2 \]
\[ + \int dS \cdot \delta \Psi^* \nabla \Psi. \]

Here, \( S \) is the outward-pointing surface normal. In the usual analysis, one assumes that \( \Psi \) and \( \nabla \Psi \) vanish at infinity, drops the boundary terms, and Eq. (1) is obtained by varying \( E - \mu N \). However, the existence of these surface terms is essential for the inclusion of higher-order interactions as discussed below.

In the rest of this paper we use trap units, \( \hbar \omega = b = 1 \), i.e., energies \( (E, V, \mu, \epsilon) \) are measured in units of \( \hbar \omega \) and lengths \( (a, r_a, r, \text{etc.}) \) in units of \( b \). Note that \( g_2 \) has dimension of length squared.

### III. THOMAS-FERMI APPROXIMATION

Let us briefly review the standard Thomas-Fermi approximation \[1, 2, 3, 4\]. Neglecting the kinetic-energy term, as compared to the trap and interaction energies, the GP equation has the solution
\[ \rho_{TF} = \frac{1}{4\pi a} \left( \mu_{TF} - \frac{1}{2} x^2 \right), \]
(6)
with chemical potential \( \mu_{TF} \). This solution is used out to the surface, \( R_{TF} \), while outside \( \rho_{TF} = 0 \). The normalization and surface condition \( \rho_{TF}(R_{TF}) = 0 \) give
\[ \mu_{TF} = \frac{1}{2} R_{TF}^2, \quad R_{TF} = (15Na)^{1/5}. \]
(7)
The total energy becomes
\[ \frac{E_{TF}}{N} = \frac{5}{7} \frac{R_{TF}^2}{2}. \]
(8)
The trap and interaction energies are \( E_V = 3E/5 \) and \( E_I = 2E/5 \), respectively. Since \( R_{TF} > 0 \) in Eq. (7), these results only hold for \( a > 0 \). The TF approximation is good for \( Na \gg 1 \), except at the surface region where the kinetic-energy density diverges. Here, the solution can be corrected as in \[2, 3, 5, 6\], essentially giving a small exponential tail.

### Inclusion of higher-order interactions

We now consider the TF approximation with the higher-order interaction term, \( \epsilon_{I2} \). Ignoring the boundary terms in Eq. (6), the modified GP equation can then be written in terms of the density \( \rho(r) = |\Psi(r)|^2 \) as
\[ \mu = \frac{1}{2} x^2 + 4\pi a \left( \rho + g_2 \nabla^2 \rho \right). \]
(9)

With scaled coordinate \( x = r/\sqrt{g_2} \) (assuming \( g_2 > 0 \) for the moment) and density \( f(r) = 4\pi a x \rho(r)/g_2 \), this becomes
\[ \frac{d^2 f}{dx^2} + f = \mu \frac{x}{g_2} - \frac{x^3}{2}, \]
(10)
The inhomogeneous and homogeneous solutions with boundary condition \( f(0) = 0 \) are
\[ f_i(x) = \left( \frac{\mu}{g_2} - \frac{1}{2} x^2 + 3 \right) x, \quad f_h(x) = \frac{A}{g_2} \sin x, \]
(11)
where \( A \) is a constant (with dimensions of length squared) to be determined later. The full solution is
\[ \rho(x) = \frac{g_2}{2\pi a} \left[ \frac{\mu}{g_2} - \frac{1}{2} x^2 + 3 + \frac{A \sin x}{g_2} \right]. \]
(12)

For a given \( A \), the chemical potential \( \mu \) and the condensate radius \( R \) are determined by the normalization and the surface condition,
\[ \int_0^{x_0} 4\pi x^2 \rho(x) \, dx = N \quad \text{and} \quad \rho(x_0) = 0, \]
(13)
where \( x_0 = R/\sqrt{g_2} \). The solution \( \rho \) should be positive for \( x < x_0 \) which must be explicitly checked. Outside \( x_0 \), we use \( \rho = 0 \).

We now consider the boundary terms in Eq. (6). Above, we assumed that \( \rho(x_0) = 0 \) at some finite radius \( x_0 \) which we identify as the condensate size. However, only the first two boundary terms in Eq. (6) vanish on account of this condition. For the last term in Eq. (6) to vanish we need \( \nabla \Psi(x_0) = 0 \), which implies that
\[ \frac{d\rho}{dx}(x_0) = 0. \]
(14)

Notice that this latter derivative is in fact non-zero in the \( g_2 = 0 \) case, which is the root of the divergence of the kinetic energy at the condensate surface as we discuss later. Equation (14) gives a closed expression for the remaining free parameter \( A \),
\[ \frac{A}{g_2} = \frac{x_0^3}{x_0 \cos x_0 - \sin x_0}. \]
(15)

This additional requirement on the derivative at the edge of the condensate implies that higher-order terms require a smoothing at the surface of the cloud. In addition, the discussion of which kinetic operator structure
to use (|∇Ψ|^2 or Ψ*∇^2Ψ) is obsolete in our treatment since the boundary term δΨ*∇Ψ vanishes. In this sense the inclusion of a higher-order term neatly removes some of the difficulties of the traditional TF treatment.

The solutions with a finite boundary R of the modified GP equation only minimize the energy functional if Eq. (14) holds. We note that extremal states of the energy functional always satisfy the virial theorem. Thus, enforcing the virial theorem on the GP solutions is equivalent to Eq. (14). We show in the Appendix that the virial theorem approach also leads to Eq. (15).

IV. SIZE AND CHEMICAL POTENTIAL

We now determine the condensate size R and chemical potential µ. The normalization condition is

\[ \frac{Na}{g_2^{5/2}} = x_0^3 \left( \frac{\mu}{3g_2} - \frac{x_0^2}{10} \right), \tag{16} \]

while the surface condition reads

\[ \frac{\mu}{g_2} - x_0^2/2 + 3 \frac{A \sin x_0}{g_2 x_0} = 0. \tag{17} \]

Combining eq. (16) - (17) gives

\[ \frac{Na}{g_2^{5/2}} = x_0^3 \left( \frac{x_0^2}{15} - 1 + \frac{x_0^2/3}{1 - x_0 \cot x_0} \right), \tag{18} \]

which determines R for given Na and g_2, and upon back-substitution also µ.

The g_2 < 0 case can be worked out analogously by replacing trigonometric functions with hyperbolicos and keeping track of signs. The two cases can in fact be combined into one equation

\[ \frac{Na}{g_2^{5/2}} = |x_0|x_0^2 \left( \frac{x_0^2}{15} - 1 + \frac{x_0^2/3}{1 - |x_0 \cot x_0|} \right). \tag{19} \]

This equation determines x_0^2 = R^2/g_2 implicitly as function of Na/g_2^{5/2}. The result is shown in Fig. 1. We notice that in principle, R becomes a multi-valued function. However, all the higher solutions for g_2 > 0 [dotted in Fig. 1] are spurious, since the density becomes negative on one or more intervals inside R. The non-spurious solutions [solid line in Fig. 1] define R as a single-valued function of a and g_2, which was not guaranteed a priori. The four quadrants in Fig. 1 correspond to the different sign combinations of a and g_2. The sign of the extra interaction energy, E_{I2}, is determined by a g_2 N^2 ρ. For a typical concave density, the Laplacian term will be negative. We therefore see that for a g_2 > 0, the higher-order interaction is attractive, whereas for a g_2 < 0, it is repulsive. The TF solution only exists for a g_2 < 0. We discuss both cases separately below.

A. The attractive regime: a g_2 > 0

For a < 0, g_2 > 0 [third quadrant in Fig. 1] there are no solutions, which is expected since the normal TF approximation has no solutions for a < 0 as the interaction energy E_I is negative and the kinetic energy that could prevent collapse is neglected.

The g_2 > 0, a > 0 case in the first quadrant has only spurious solutions. Here the g_2 term is attractive for the typical concave density and a collapse towards a high-density state is possible in complete analogy to the usual discussion of attractively interacting condensates within the standard GP theory. Whereas there can be metastable states at large values of Na/g_2^{5/2}, these are stabilized by kinetic energy and thus are not present in our TF approach. Thus, even when the total kinetic energy is small, it is still needed to prevent the attractive higher-order term from amplifying local-density variations.

This important point can also be established by considering the stability of the homogeneous condensate through linearization of the GP equation. By repeating the analysis of [2] with the higher-order term, we find that for g_2 > 0 and a > 0, the kinetic-energy term is crucial for the stability of the excitation modes. In fact, exponentially growing modes will always be present if the kinetic energy is neglected. This will be discussed elsewhere in relation to the numerical solution of the full GP equation [13].
was expected since a/ \(\rightarrow\) evolution approaches the normal TF result in Eq. (7) when \(a/\) which connects smoothly to the (a) solution. In the limit lower part of (b) has \(\mu > 0\). The lower part of (b) has \(\mu < 0\). Points indicate data from Tab. I. All values are in trap units.

\[\text{FIG. 2: (Color online) Chemical potential} \mu \text{ as function of} Na \text{ and} g_2 \text{ as found in the modified TF approximation, using the solutions (a) and (b) from Fig.}\ \text{For branch (a) and the upper part of branch (b) (see inset), we have} \mu > 0. \text{The lower part of (b) has} \mu < 0. \text{Points indicate data from Tab. I. All values are in trap units.}\]

\[\text{V. DENSITIES AND ENERGIES}\]

With \(R\) and \(\mu\) determined, we can find the density profile, energy densities and integrated energy contributions. With Eq. (12), the energy densities are given by

\[\epsilon_V = \frac{x^2}{2} \rho, \quad \epsilon_I = 2\pi a \rho^2, \quad (20)\]

\[\epsilon_I = -\frac{1}{2} \rho \left(3 + \frac{4}{g_2} \sin x\right). \quad (21)\]

Using Eq. (9), the total energy density (without \(\epsilon_K\)) becomes

\[\epsilon \equiv \epsilon_V + \epsilon_I + \epsilon_{I2} = \frac{1}{2} \rho(x)(V(x) + \frac{\mu}{g_2}). \quad (22)\]

In Fig. 3 we show the density profile of the (a) solutions for \(Na = 10^4\) and selected \(g_2 < 0\). We clearly see that the higher-order term tends to expand the condensate through its repulsion. Importantly, at the boundary, there is a smoothing caused by the condition in Eq. (14) [see inset in Fig. 3]. We will discuss how this affects the estimated kinetic energy in the next section. As \(|g_2|\) grows, we see the condensate flatten and in the limit of very large \(|g_2|\), it becomes a constant density.

\[\text{FIG. 3: (Color online) Densities for branch (a) in Fig.}\ \text{We clearly see that the higher-order term tends to expand the condensate through its repulsion. Importantly, at the boundary, there is a smoothing caused by the condition in Eq. (14) [see inset in Fig. 3]. We will discuss how this affects the estimated kinetic energy in the next section. As \(|g_2|\) grows, we see the condensate flatten and in the limit of very large \(|g_2|\), it becomes a constant density.}\]
In the TF approximation, the release energy is simply the kinetic term. Since we neglect the kinetic term, it is very large near the boundary as in the usual TF approximation, so the kinetic energy will be strictly zero at $R$. However, as one approaches the boundary, the kinetic-energy density grows rapidly before it descends towards zero within a very small interval at $R$. The total energy density in Eq. \ref{eq:22} goes to zero at this point and we find that $\epsilon_K/\epsilon$ is very large near the boundary as in the usual $g_2 = 0$ case.

We now address the validity of the TF approximation with the $g_2$ term included. In order to do so, we must consider the contribution of the kinetic energy. The kinetic energy density can be written as

$$\epsilon_K = \frac{g_2}{8\rho(4\pi a)^2} \left( x + \frac{A x \sin x - \cos x}{g_2} \right)^2. \quad (23)$$

Strictly speaking, this is not the true kinetic energy, since the kinetic terms were neglected from the start. However Eqs. \ref{eq:22} and \ref{eq:23} can be used to test whether the TF approximation holds locally, i.e., $\epsilon_K \ll \epsilon$ should hold for the solution $\rho$ to be consistent. In Tab. \ref{tab:1} we calculate the integrated contribution of the kinetic energy relative to the total TF energy and we find that the contribution is small everywhere except the point where $E = 0$ on the $g_2 > 0$ side of Fig. \ref{fig:5} here, the kinetic energy is of course the most important term and the TF approximation is poor.

In the standard TF, the kinetic energy causes trouble at the boundary of the cloud. Here, $\nabla \Psi \propto \nabla \rho/\sqrt{\rho}$ and since the density vanishes and the derivative is finite [see Eq. \ref{eq:6}], this diverges at $R_{TF}$. When including the higher-order term we need to use the additional boundary condition $\nabla \Psi = 0$ at $R$, so the kinetic energy will be strictly zero at $R$. However, as one approaches the boundary, the kinetic-energy density grows rapidly before it descends towards zero within a very small interval at $R$. The total energy density in Eq. \ref{eq:22} goes to zero at this point and we find that $\epsilon_K/\epsilon$ is very large near the boundary as in the usual $g_2 = 0$ case.

We conclude that the inclusion of the higher-order term does not alleviate the difficulties with kinetic energy at the boundary. The techniques for addressing this problem described in \ref{sec:6} should therefore be generalized to include the higher-order interaction term in order to improve the description at the boundary of the cloud.

### VII. COMPARISON TO ATOMIC SYSTEMS

The considerations above show that deviations from the usual TF approximation can be strong when $g_2$ is large. In the following, we reintroduce explicit units for comparison with real systems. We have to consider $g_2/b^2$.
Of course, the $b^2$ factor means that this quantity is generally very small since $g_2$ is of order $a_0^3$ and $b$ is of order $10^{4}a_0$.

We first consider some typical background values for bosonic alkali atoms away from resonance. We estimate the effective range to be the of order of the potential range and assuming a van der Waals interaction, we have $r_e \sim 50 - 200a_0$. For typical one-component gases we have $-450a_0 \lesssim a \lesssim 2500a_0$. Since $g_2 = a^2/3 - ar_e/2$, we see that the $a^2$ term will dominate and in all cases $0 < g_2 \lesssim 10^6a_0$. In trap units, this becomes $g_2/b^2 \lesssim 5 \cdot 10^{-3}(1\mu m/b)^2$. In typical traps of $b \sim 1 - 10\mu m$, the higher-order term is therefore very small. These values also predominantly lie in the first quadrant of Fig. 1 and thus no TF solution exists.

Let us first consider Feshbach resonances in order to increase the influence of the $g_2$ term. We use a multi-channel Feshbach model [17], which describes the full $T$ matrix as a function of resonance position $B_0$, width $\Delta B$, magnetic-moment difference between the channels $\Delta \mu$, and the background scattering length $a_{bg}$. Performing an effective-range expansion [11], we have $a = a_{bg}[1 - \Delta B/(B - B_0)]$ and $r_e = r_{e0}/[1 - (B - B_0)/\Delta B]^2$, where $r_{e0} = -2\hbar^2/ma_{bg}\Delta \mu\Delta B < 0$. Combining these relations, we find $r_e = r_{e0}(1 - a_{bg}/a)^2$ and

$$g_2(a) = \frac{a^2}{3} - \frac{ar_{e0}}{2}(1 - \frac{a_{bg}}{a})^2.$$ (24)

Hence $g_2$ diverges when $a \to 0$ (referred to as zero-crossing) or $a \to \infty$ (on resonance). Near zero-crossing, the effective-range expansion is, however, severely divergent and its validity is questionable. Even so, the effective-range corrections near zero-crossing obtained are in fact identical to those obtained from use of the full T-matrix [18]. One finds $\lim_{a \to 0} ag_2 = |r_{e0}|a_{bg}^2/2$, where $r_{e0} < 0$.

As a concrete example, we consider the alkali isotope $^{39}$K where several Feshbach resonances of vastly different widths were found recently [19]. First, we focus on zero-crossing and consider the very narrow resonance at $B_0 = 28.85G$ with $\Delta B = -0.47G$, $\Delta \mu = 1.5\mu B$, and $a_{bg} = -33a_0$. We obtain $r_{e0} = -5687a_0$ and $ag_2 \to 93.8 \cdot 10^3a_0^3$ for $a \to 0$. It is important to notice that $ag_2 > 0$ around $a = 0$. This means that we are looking for solutions in the first and third quadrants of Fig. 1 and again we have to conclude that no TF solutions can be found when higher-order terms are taken into account.

Another case of interest is around resonance where $|a| = \infty$. Here, we have $r_e \sim r_{e0}$ and $g_2 \propto a^2 > 0$ on both sides of the resonance. Thus, the $a > 0$ side will be in the first and the $a < 0$ in the second quadrant of Fig. 1. This makes it difficult to imagine sweeping the resonance from either side to probe the solutions on branch (b) in Fig. 1. One could imagine starting on the $a > 0$ side with small $g_2 > 0$. The full GP equation will have perfectly sensible solution here, however, when one approaches the resonance the $g_2$ term will diverge and induce collapse already on the $a > 0$ side. If we approach from the $a < 0$ side, then we face the problem that the critical number of particles decreases dramatically before $g_2$ grows sufficiently and one therefore needs a very small condensate since $Na/B \sim 0.5$ [11]. At this point, the TF approximation is no longer valid.

The Feshbach resonance used to increase $g_2$ must be very narrow in order for $r_{e0}$ to be large. However, most experimentally known resonances are not narrow. For broad or intermediate resonances, we have to consider the long-range van der Waals interaction when calculating the effective-range corrections. Analytic formulas for this case have been worked out in [20], and we note that the effective range diverges as $a^2$ near zero crossing exactly as in the Feshbach model above. For very narrow

| $g_2$ | $R$ | $\mu$ | $E_V/N$ | $E_I/N$ | $E_{12}/N$ | $E/N$ | $E_R/N$ | $E_K/E$ |
|-------|-----|-------|---------|---------|-----------|-------|--------|--------|
| (a)   | −0.1| 10.9447 | 58.8188 | 25.2164 | 16.7865 | 0.01465 | 42.0176 | 16.8012 | 1.8\times 10^{-3} |
| (b)   | 50 b| 15.407 | 63.0102 | 38.9723 | 8.92496 | 29.0439 | 50.9912 | 12.0189 | 0.43\times 10^{-3} |
| (c)   | 1.0 | 14.480 | 327.612 | 3.04199 | 416.359 | 251.032 | 66.7542 | 21.0706 | 0.30\times 10^{-3} |

The kinetic energy estimated by surface corrections as in [2].

The total energy $|E|$ is zero near $g_2 = 5.14$, hence the TF approximation is invalid here.

TABLE I: Chemical potential $\mu$ and condensate size $R$ for different $g_2$ and fixed $N|a| = 10^4$. The integrated energies are trap ($E_V$), interaction ($E_I$, $E_{12}$), total ($E = E_V + E_I + E_{12}$), and release energy ($E_R = E - E_V$). The TF limit is approached for $g_2 \to 0$. The ratio of kinetic energy $E_K$ to total energy $E$ indicates where the TF approximation is valid. The corresponding density distributions are shown in Figs. 3 and 4. All values are in trap units.
resonances, we still have $\beta_6 < r_{\text{c0}}$, where $\beta_6$ is the characteristic length of the van der Waals interaction. The model above should thus give the dominant contribution.

Using the van der Waals formulas we can estimate $ag_2$ at zero crossing. We find

$$\frac{ag_2}{b^3} \sim \frac{1}{3x_c} \left( \frac{\beta_6}{b} \right)^3,$$  \hspace{1cm} (25)

where $x_c = (\Gamma[1/4])^2/2\pi$, with $\Gamma$ the gamma function. We have explicitly introduced the oscillator length which is the relevant length scale of comparison. Importantly, we find that $ag_2 < 0$ for $a > 0$ and we are thus in the fourth quadrant where a TF solution exists. For $a < 0$, we pass to the second quadrant as $g_2$ becomes positive and a single collapsed solution can be found.

We now estimate the parameters obtained from the van der Waals formulas. With $b = 1\mu$m and $\beta_6 \sim 123.3a_0$ [2], we have $ag_2/b^3 \sim -10^{-8}$. We thus have $Na/g_2^{3/2} \propto 10^7(Na)a^{-1/2}$. For values of $a$ that are not extremely small, the solution is therefore typically located far to the right in Fig. 1 where it will look similar to the $g_2 = 0$ case. We can estimate how close to zero one would have to tune $a$ in order to see deviations using the $a \to 0$ limit of the van der Waals effective range. Let us aim for $g_2/b^2 = -10$ which should be observable in the condensate profile according to Fig. 4. With $b = 1\mu$m, we need $a \sim 10^{-6}\beta_6 \sim 1.7 \times 10^{-4}a_0$. Using broad resonances, one can tune to zero at the level of $10^{-2}a_0$ in $39\text{K}$. Observing the effect of the $g_2$ term therefore seems out of reach at the moment, but might be possible in the near future. Of course, we still have to maintain a large value of $Na$ for kinetic energy to be small, and thus a larger condensate is needed close to zero crossing.

From the examples above, we see problems in accessing the TF solutions presented above in current experiments with ultracold alkali gases. In particular, we notice that realistic systems which have been used for creation of BECs in alkali-metal gases for the last decades have parameters that predominantly lie in the first quadrant of Fig. 1. As we have discussed, there are no well-defined TF solutions in that region. Therefore, we see that the kinetic energy plays a decisive role and we are forced to consider it in principle, even if it is small for all practical purposes. The physical reason is that for $a > 0$ and $g_2 > 0$, the higher-order interaction is effectively attractive and induces collapse which will have to be balanced by a barrier from the kinetic term, similar to the $a < 0$, $g_2 = 0$ case [1]. Since we neglect the kinetic term in the TF approximation, we should not expect to find solutions in the $ag_2 > 0$ case.

Only in the case of resonances dominated by the long-range van der Waals interaction do the parameters allow for TF solutions with non-zero $g_2$. However, here the length scale of the trap makes the contribution very small and the TF solution becomes identical to the $g_2$ case. One could in principle tune $a$ very close to zero-crossing and obtain a significant contribution but the level of tuning required is beyond current experimental reach.

VIII. CONCLUSIONS

We have considered the effect of higher-order interactions in Bose-Einstein condensates within the Gross-Pitaevskii theory. We derived the GP equation with effective-range corrections included and solved it analytically in the Thomas-Fermi approximation. Higher-order interaction terms act as derivatives on the condensate wave function which means that the boundary conditions on the solutions of the GP equation must be carefully considered. We then discussed the solutions for various parameters and presented the chemical potential, density profiles, and the energy contributions.

We find that no TF solutions are possible when the higher-order term is attractive. This conclusion holds both in the trapped system and in the homogeneous case [15]. An estimate of the relevant parameters for alkali atoms showed that away from resonances, they typically lie in the region where the effective-range correction is effectively attractive and likewise near very narrow Feshbach resonances. We conclude that in those cases, the kinetic energy, even if very small, is crucial in order to stabilize collapse due to higher-order interaction terms. For broader resonances where the long-range van der Waals potential is dominant, we find that modified TF solutions exist. However, for typical traps, the parameters are very small and tuning of the scattering length near zero crossing at a level beyond current experimental reach is necessary. This might of course become possible as experimental control improves in the future.

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APPENDIX A: DETERMINATION OF $A$ FROM THE VIRIAL EQUATION

Even though Eq. (12) is a solution to the modified GP equation Eq. (9) for all $A$, it does not necessarily minimize the energy functional as discussed in the main text. This can also be seen from the virial equation (with neglected kinetic energy),

$$-2E_V + 3E_I + 5E_{12} = 0,$$  \hspace{1cm} (A1)

which holds for all extremal points of the energy functional. Equation (A1) is derived from the energy functional using scaling arguments as in [2].

As an example, consider the $A = 0$ solution in Eq. (12). This solution has a chemical potential shifted by $3g_2$ compared to the $g_2 = 0$ TF result. But the density is unchanged and so is $E_V$ and $E_I$. Hence, the usual virial equation $-2E_V + 3E_I = 0$ for $g_2 = 0$ also holds for $g_2 \neq 0$. Since $E_{12} = -3g_2/2 \neq 0$, the virial equation Eq. (A1) is not fulfilled, and hence the $A = 0$ solution is not extremal. Below, we use the virial equation to calculate the value of $A$ that minimizes the energy functional and the corresponding $R$ and $\mu$. We will also
prove that this condition is in fact equivalent to assume \( \rho(x_0) = \nabla_x \rho(x_0) = 0 \) at the boundary.

The general results for \( A \), \( R \), and \( \mu \) can be derived using the normalization and surface conditions Eq. (13), and the virial equation Eq. (A1). For convenience, we introduce the variables \( \bar{\mu} = \mu / (3g_2) + 1 \), \( \bar{A} = A / (3g_2) \), and \( c = Na / g_2^{5/2} \). The different energy contributions are

\[
E_V = 3s \int_0^{x_0} dx x^4 \left( \bar{\mu} - \frac{x^2}{6} + \bar{A} \sin \frac{x}{x} \right),
\]

\[
E_I = 9s \int_0^{x_0} dx x^2 \left( \bar{\mu} - \frac{x^2}{6} + \bar{A} \sin \frac{x}{x} \right)^2,
\]

\[
E_{I2} = -9s \int_0^{x_0} dx x^2 \left( \bar{\mu} - \frac{x^2}{6} + \bar{A} \sin \frac{x}{x} \right) \left( 1 + \bar{A} \sin \frac{x}{x} \right),
\]

(A2)

where \( s = g_2^{7/2} / (2a) \). Direct integration of Eq. (A2), insertion of \( \bar{\mu} \) from Eq. (17), and some algebra gives the virial equation

\[
0 = -2E_V + 3E_I + 5E_{I2}
\]

\[
= -\frac{s}{x_0} \left( x_0^2 - 3\bar{A}(x_0 \cos x_0 - \sin x_0) \right)^2.
\]

(A3)

We immediately see that this is in fact equivalent to Eq. (15). Therefore, the solution we have explicitly found above minimizes the energy functional with boundary conditions \( \rho(x_0) = \nabla_x \rho(x_0) = 0 \). More generally, when we solved the modified GP equation without considering the boundary terms in Sec. (III), we found a one-parameter family of solutions (parametrized by \( A \)). The virial theorem is merely a constraint on \( A \) for obtaining a minimum of \( E \).

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