

# Simple model for interactions and corrections to the Gross-Pitaevskii equation

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One of the assumptions leading to the Gross-Pitaevskii equation (GPE) is that the interaction between atom pairs can be written effectively as a  $\delta$  function so that the interaction range of the particles is assumed to vanish. A simple model that takes into account the extension of the interparticle potential is introduced. The correction to the GPE predictions for the energy of a condensate confined by a harmonic trap in the Thomas-Fermi regime is estimated. Although it is found to be small, we believe that in some situations it can be measured using its dependence on the frequency of the confining trap. Due to the simplicity of the model, it may have a wide range of applications.

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## I. INTRODUCTION

The ground state of a weakly interacting Bose-Einstein condensate (BEC) satisfies the Gross-Pitaevskii equation (GPE) [1,2]

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U(r)\psi + Ng_{3D}|\psi|^2\psi = \mu\psi, \quad (1)$$

where  $U(r)$  is an external confining potential,  $\mu$  is the chemical potential,  $N$  is the number of atoms, and  $g_{3D} = 4\pi\hbar^2 a/m$  is nonlinearity strength for the  $s$ -wave scattering length  $a$ . The wave function  $\psi$  is normalized to 1. In this work, we use a modified one-dimensional version of GPE that will be derived in the next section.

Despite its simplicity, the GPE describes many experiments and became very popular in the cold atoms community. The derivation of the GPE [1,3] relies on two assumptions. The first is the mean-field approximation, i.e., all atoms have the same wave function, so we may write the total wave function  $\Psi(x_1, x_2, \dots, x_N)$  for  $N$  atoms as a product of single-particle wave functions  $\psi(x_i)$ ,

$$\Psi(x_1, x_2, \dots, x_N) = \prod_{i=1}^N \psi(x_i). \quad (2)$$

The second assumption is that the interaction between atoms can be replaced by a contact interaction

$$V(\vec{r}_1 - \vec{r}_2) = g_{3D}\delta(\vec{r}_1 - \vec{r}_2), \quad (3)$$

with the  $\delta$  function appropriately introduced via the pseudopotential theory [4]. In this work, the validity of this approximation and possible situations where the approximation (3) is not justified are studied. For this purpose we remember that in the derivation of the GPE (1) the origin of the terms nonlinear in  $\psi$  is the Hartree term [1,2],

$$E_H = \int d\vec{r}_2 d\vec{r}_1 |\psi(\vec{r}_1)|^2 V(\vec{r}_1 - \vec{r}_2) |\psi(\vec{r}_2)|^2. \quad (4)$$

If one can assume that the variation of the wave function is small over the regime where the potential  $V(\vec{r}_1 - \vec{r}_2)$  is

substantial, we can approximate  $|\psi(\vec{r}_2)|^2$  by  $|\psi(\vec{r}_1)|^2$ . In this case, the effective potential (3) can be used (this should be done with care [1,2,4] but in one dimension, it is trivial). In general, the term (4) makes the calculations more involved. In the present work we are interested in the exploration of the qualitative difference between the ground-state energy in contact potentials where the particles can be considered pointlike and realistic potentials where the range of the interaction potential is not negligible. Neutral atoms interact via the van der Waals interaction, and the extension of the potential is often comparable to the van der Waals radius [5], and related to effective range in scattering theory. It is usually much larger than the Bohr radius or the “size” of the atom. To study this effect we introduce (in Sec. II) a model potential and show how it can be written as a one-dimensional potential consisting of three  $\delta$  functions separated by a characteristic length. The middle one models the repulsion while the outer ones model the attraction. For the sake of simplicity we study a one-dimensional model, namely we study the corrections to (1) in an elongated trap. We believe that similar effects will be found also in higher dimensions of the trap. We are interested in weakly interacting BECs at zero temperature with a time-independent harmonic trapping potential. The ground-state density (including corrections related to nonvanishing range of interaction) is presented in Sec. III and corrections to the energy are calculated in Sec. IV and given by Eq. (48) which is the main result of this work. The magnitude of the correction is estimated and the results are discussed in Sec. V.

## II. MODIFIED GPE FOR $\delta$ -FUNCTIONS INTERACTION

We would like to write a toy model for three-dimensional interactions in a one-dimensional trap. Let us replace the usual GPE interaction term (3) by

$$V(r) = \begin{cases} \frac{3(g_{3D} + \lambda)}{4\pi r_{in}^3} & \text{for } r < r_{in} \\ -\frac{\lambda}{4\pi r_{out}^2 \epsilon_{out}} & \text{for } r_{out} < r < r_{out} + \epsilon_{out} \\ 0 & \text{otherwise} \end{cases}, \quad (5)$$

where  $r \equiv |\vec{r}_1 - \vec{r}_2|$ , the coupling constant between particles is  $g_{3D} > 0$ , and  $\lambda > 0$  is the strength of noncontact attraction interactions.  $r_{\text{out}}$  is a length scale which determines the interaction range, while  $r_{\text{in}}$  is a much smaller length scale ( $r_{\text{in}} \ll r_{\text{out}}$ ). We take the limit  $r_{\text{in}}, \varepsilon_{\text{out}} \rightarrow 0$  while  $r_{\text{out}}$  is fixed. This model does not require the use of a pseudopotential and is similar in spirit to the introduction of a pseudopotential. The potential (5) is composed of repulsive and attractive terms, like the van der Waals potential, and therefore captures the physics of van der Waals interaction without giving up the mathematical and numerical simplicity. The simplicity results from the fact that in the limit  $r_{\text{in}} \rightarrow 0$  and  $\varepsilon_{\text{out}} \rightarrow 0$ , the potential (5) is effectively a sum of  $\delta$  functions.

According to [6], it is possible to formulate a modified GPE which takes the range of the pair interaction into account, as follows. For  $\lambda = 0$  one finds the standard GPE (1). The contribution due to the nonvanishing size of the particles  $r_{\text{out}}$  was found by Collin, Massignan, and Pethick [6] (for earlier work see [7]). In our case it takes the form

$$\Delta E_{\text{int}} = -Ng_{3D}g_2k^2|\psi(k)|^2 = N\left(\frac{2\lambda}{3}r_{\text{out}}^2\right)k^2|\psi(k)|^2, \quad (6)$$

where  $\hbar k$  is the relative momentum of the colliding particles. Here  $g_2 = a(\frac{1}{3}a - \frac{1}{2}r_e)$  where  $r_e$  is the effective range of the interaction and the result of the calculation in Appendix A [Eq. (A15)] was used. In coordinate space, the resulting equation is [6]

$$\mu\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + U(r)\psi + Ng_{3D}|\psi|^2\psi + Ng_{3D}g_2\nabla^2|\psi|^2\psi. \quad (7)$$

The leading correction to the GPE does not depend on the details of the interparticle potential, therefore we can study the effect of the corrections in terms of our simplified potential (5).

Since the trap is one dimensional, we wish to use a one-dimensional wave function  $\psi(x)$  rather than  $\psi(\vec{r}) = \psi_x(x)\psi_y(y)\psi_z(z)$ . For this purpose, we integrate (7) over the transverse directions  $y$  and  $z$ , resulting in

$$\mu\psi_x(x) = E_{\perp}\psi_x(x) - \frac{\hbar^2}{2m}\frac{d^2\psi_x(x)}{dx^2} + U(x)\psi_x(x) + g|\psi_x(x)|^2\psi_x(x) + g'g_2\frac{d^2|\psi_x(x)|^2}{dx^2}\psi_x(x), \quad (8)$$

where

$$g = Ng_{3D}\frac{m\omega_{\perp}}{2\pi\hbar}\left[1 - 2g_2\frac{m\omega_{\perp}}{\hbar}\right] \quad (9)$$

and

$$g' = Ng_{3D}\frac{m\omega_{\perp}}{2\pi\hbar}. \quad (10)$$

Here  $\omega_{\perp}$  is the (high) frequency of the confining trap in the directions perpendicular to the BEC line. In the present work we consider the regime where the confining frequency  $\omega_{\perp}$  is sufficiently high so that the energies are lower than the first excited state of the transverse motion, but is sufficiently low so that the width of the ground state in the transverse direction,  $a_{\perp}$ , is much larger than the three-dimensional scattering length  $a$ . Different physics is expected in the opposite regime where

the requirement  $a \ll a_{\perp}$  is not satisfied (see [8]). Since  $g_2$  is typically small, we are allowed to neglect terms of the second order in  $g_2$  and replace  $g'$  by  $g$  in Eq. (8). We would like to write a one-dimensional GPE with the interparticle potential

$$V(x) = 2g\delta(x) - \frac{1}{2}g[\delta(x+l) + \delta(x-l)], \quad (11)$$

where  $l$  is the effective extension of the interparticle potential to be related to the parameters  $r_{\text{out}}$ ,  $g_{3D}$ , and  $\lambda$  of potential (5); see Appendix A. The one-dimensional nonlinearity constant  $g$  is related to  $g_{3D}$  by (9) and (10). Since the density does not change much on the length scale  $l$ , the GPE (1) modified by the replacement  $g\delta(x) \rightarrow V(r)$  of (5) and eventually by  $V(x)$  of (11) can be written as

$$\mu\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) + g|\psi(x)|^2\psi(x) - \frac{1}{2}gl^2\frac{d^2|\psi(x)|^2}{dx^2}\psi(x). \quad (12)$$

Taking the limit  $l \rightarrow 0$ , we recover the standard one-dimensional GPE. To establish the relation with three-dimensional energy correction, we compare between Eqs. (8) and (12) and replace  $g'$  by  $g$  resulting in

$$\frac{1}{2}l^2 = -g_2 = -a\left(\frac{a}{3} - \frac{r_e}{2}\right). \quad (13)$$

Using more realistic interaction functions (for example, a continuous potential) generalizes and replaces the coefficient  $l^2$  in Eq. (12) by a model dependent constant  $g_2$ . Hereafter, we consider only the simple model (11). Nevertheless, our results are valid for any short-range interaction. In other words, we demonstrate the dependence of the corrections on the range of the interparticle potential.

Here, we add an extra term of the order of  $\text{const} \times a^3k^2$  to the standard GPE [see for example (6) where  $r_{\text{out}}$  is of order  $a$  and  $\lambda$  is of the same magnitude as  $g$  which is proportional to  $a$ ]. Note that taking into account contributions from components of higher angular momentum in the partial waves expansion will also add extra terms to the GPE. The magnitude of these terms is of the order of

$$E_{\mathcal{L}} \sim \text{const} \times a^{2\mathcal{L}+1}k^{2\mathcal{L}} \quad (14)$$

as derived in Appendix B of [4], where  $\mathcal{L}$  is the quantum number of angular momentum. Hence,  $s$ -wave interaction contributes energy of order  $a$  (without the correction (6)) and  $p$ -wave interaction contributes energy of order  $\text{const} \times a^3k^2$ . However, for spinless bosons,  $p$ -wave interaction is forbidden (because it is antisymmetric with respect to interchange of two bosons, see [9]). Therefore, the correction (6) presented here for the GPE is more significant than corrections originating from higher orders of partial waves expansion.

### III. GROUND STATE OF A THOMAS-FERMI (TF) BEC IN A HARMONIC TRAP

We would like to compare the ground states of the standard GPE (1) and the modified GPE (12) in a time-independent trapping potential  $U(x)$ . The Thomas-Fermi (TF) approximation [3] for the standard GPE (where the kinetic energy is

neglected) is

$$U(x)\psi(x) + g|\psi(x)|^2\psi(x) = \mu\psi(x). \quad (15)$$

Introducing the density  $\rho_0 = |\psi(x)|^2$ , it takes the form

$$\rho_0 = \frac{1}{g}[\mu - U(x)], \quad (16)$$

where  $\mu$ , the chemical potential, is a constant determined by the normalization  $\int_{-R}^R |\psi(x)|^2 dx = 1$  and  $R$  satisfies

$$\mu = U(r). \quad (17)$$

The TF approximation is valid at the central region of the trap,  $-R \lesssim x \lesssim R$  [10]. For a harmonic trap

$$U(x) = \frac{1}{2}m\omega^2 x^2. \quad (18)$$

Normalization of the wave function,  $\int_{-R}^R |\psi|^2 dx = 1$ , yields

$$\mu = \left( \frac{3\sqrt{m}}{2^{5/2}} g\omega \right)^{2/3} \quad (19)$$

and

$$R = \sqrt{\frac{2\mu}{m\omega^2}} = \left( \frac{3}{2m} g\omega^{-2} \right)^{1/3}. \quad (20)$$

In what follows, this value of  $R$  (that is independent of  $l$ ) will be used. The chemical potential for the standard GPE, defined as

$$\mu = \int \left[ -\psi^* \frac{\hbar^2}{2m} \nabla^2 \psi + U(r)|\psi|^2 + g|\psi|^4 \right] dx, \quad (21)$$

is related to the various energy contributions (kinetic energy  $E_k$ , potential energy  $E_p$  and nonlinear energy  $E_{nl}$ ) by

$$\mu = E_k + E_p + 2E_{nl}. \quad (22)$$

For a harmonic potential [1, p. 167],

$$E_k - E_p + \frac{1}{2}E_{nl} = 0, \quad (23)$$

so, if  $E_k$  is negligible (as assumed in the TF approximation),

$$E_{nl} \approx 2E_p \approx \frac{2}{5}\mu \quad (24)$$

leading to

$$E_p \approx \frac{1}{5}\mu = \frac{1}{5} \left( \frac{3\sqrt{m}}{2^{5/2}} g\omega \right)^{2/3} \quad (25)$$

and

$$E_{nl} \approx \frac{2}{5}\mu = \frac{2}{5} \left( \frac{3\sqrt{m}}{2^{5/2}} g\omega \right)^{2/3}. \quad (26)$$

The total energy of a particle in the condensate is given by

$$E = \frac{3}{5}\mu = \frac{3}{5} \left( \frac{3\sqrt{m}}{2^{5/2}} g\omega \right)^{2/3}. \quad (27)$$

Now, let us consider the modified GPE (12). In the TF approximation it takes the form

$$\begin{aligned} U(x)\psi(x) + g|\psi(x)|^2\psi(x) - \frac{1}{2}gl^2 \frac{d^2|\psi(x)|^2}{dx^2} \psi(x) \\ = \mu(l)\psi(x) \end{aligned} \quad (28)$$

that reduces to [in analogy to (16)]

$$|\psi(x)|^2 - \frac{1}{2}l^2 \frac{d^2|\psi(x)|^2}{dx^2} = \frac{1}{g}[\mu(l) - U(x)] \quad (29)$$

and

$$\rho(x) = |\psi(x)|^2 \approx \frac{1}{g}[\mu(l) - U(x)] - \frac{1}{2g}l^2 \frac{d^2U(x)}{dx^2}. \quad (30)$$

A similar differential equation was studied and solved in Ref. [11] (for discussion regarding the stability of the solutions see [12]). However, we assume that the term  $\frac{1}{2g}l^2 \frac{d^2\rho(x)}{dx^2}$  in Eq. (30) can be considered as a perturbation so that for a harmonic trap (18) one finds

$$\rho(x) \approx \frac{1}{g} \left( \mu(l) - \frac{1}{2}m\omega^2 x^2 - \frac{1}{2}m\omega^2 l^2 \right). \quad (31)$$

This density differs from the standard GPE density

$$\rho_0(x) = \frac{1}{g} \left( \mu(0) - \frac{1}{2}m\omega^2 x^2 \right) \quad (32)$$

by a small negative constant

$$\rho - \rho_0 = -\Delta\rho = \frac{\Delta\mu}{g} - \frac{1}{2g}m\omega^2 l^2, \quad (33)$$

where  $\Delta\mu = \mu(l) - \mu(0)$ .

The TF approximation is valid only at the central part of the trap, where the density of atoms is very large. Since both  $\rho(x)$  and  $\rho_0(x)$  are normalized to 1, we expect that on the edges of the condensate, where the second derivative of the density is positive,  $\rho(x)$  will be higher than  $\rho_0(x)$ . The edge is defined by  $R - 2d < |x| < R$ , where  $d$ , the typical thickness of the boundary, satisfies [10]

$$\left. \frac{dU}{dr} \right|_R d = \frac{\hbar^2}{2md^2}$$

or

$$d = \left( \frac{2m}{\hbar^2} \left. \frac{dU}{dx} \right|_R \right)^{-1/3} = \left( \frac{2m^2}{\hbar^2} \omega^2 R \right)^{-1/3}. \quad (34)$$

In Sec. IV and in Appendix B,  $\Delta\rho$  is calculated [see Eq. (B29)] and is found to take the value of

$$\Delta\rho = \frac{1}{4g}m\omega^2 l^2 \quad (35)$$

resulting in

$$\Delta\mu = \frac{1}{4}m\omega^2 l^2. \quad (36)$$

It is possible to calculate both  $\rho_0(x)$  and  $\rho(x)$  numerically. Numerical determination of the ground state is generally carried out by propagating in imaginary time, i.e., one replaces  $\delta t$  with  $-i\delta t$  in the split step evolution operator and normalizes the wave function to 1 after each time step. We use the evolution operator

$$\begin{aligned} \hat{P} = \exp \left[ -\frac{\delta t}{\hbar} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) + 2g|\psi(x)|^2 \right. \right. \\ \left. \left. - \frac{1}{2}|\psi(x+l)|^2 - \frac{1}{2}|\psi(x-l)|^2 \right) \right], \end{aligned} \quad (37)$$

corresponding to the time-dependent version of (12), and stop the propagation when a steady state is reached, i.e.,

$$\hat{P}\psi = \bar{\lambda}\psi, \quad (38)$$

where the factor  $\bar{\lambda}$  (which is close to 1 for small  $\delta t$ ) is eliminated after normalization.

This scheme works better if we choose the initial wave function to be close to the ground state. We take the approximate ground state (32) as an initial wave function. Propagating the modified GPE (12) in a split-step technique with imaginary time steps minimizes the energy and gives the perturbed ground state for particles interacting with a potential of finite range. We repeat this calculation for various values of the interaction range  $l$  (including  $l = 0$ ) and see that (31) and (33) are satisfied in the central region of the trap (Fig. 1) with (35) and (36). One should distinguish between the correction to the TF approximation in the vicinity of  $x = R$  [Fig. 1(a)] and the correction resulting of the nonvanishing value of  $l$  [Figs. 1(b) and 1(c)]. Note that our analytical results are valid *only* when the TF approximation holds.

#### IV. ENERGY OF A THOMAS-FERMI BEC IN HARMONIC TRAP

The energy of a BEC according to the modified GPE (12) is a sum of kinetic, potential, and nonlinear contributions. In the Thomas-Fermi (TF) approximation, we neglect the kinetic energy and we are left with potential energy

$$E_p = \int \psi^*(x)U(x)\psi(x)dx = \int \rho(x)U(x)dx \quad (39)$$

and with interaction energy

$$\begin{aligned} E_{nl} &= \frac{g}{2} \int dx \left[ |\psi(x)|^4 - \frac{1}{2}l^2 \frac{d^2}{dx^2} |\psi(x)|^2 |\psi(x)|^2 \right] \\ &= \frac{g}{2} \int dx \left[ \rho^2(x) - \frac{1}{2}l^2 \frac{d^2}{dx^2} \rho(x) \rho(x) \right]. \end{aligned} \quad (40)$$

In the ground state of the harmonic trap with only contact interaction ( $l = 0$ ), these energies are given by (25) and (26).

The ground-state energy of the modified GPE (12)

$$E = E_p + E_{nl} \quad (41)$$

can be written in the form

$$E = E(l=0) + \Delta E(l). \quad (42)$$

Assuming that in the regime where the TF approximation holds the deviation of  $\rho$  from  $\rho_0$  is a constant denoted by  $\delta\rho$ ,  $E(l=0)$  can be considered as a minimum of

$$E_0 = E(l=0) + C_2^{\text{GP}}(\delta\rho)^2 \quad (43)$$

with respect to  $\delta\rho$ , with the constant  $C_2^{\text{GP}} > 0$  [see Appendix B, (B11)]. The ground state energy of the modified GPE is the minimum of

$$E = E(l=0) + C_2^{\text{GP}}(\delta\rho)^2 + C_0^{\text{pert}}(l) + C_1^{\text{pert}}(l)\delta\rho, \quad (44)$$

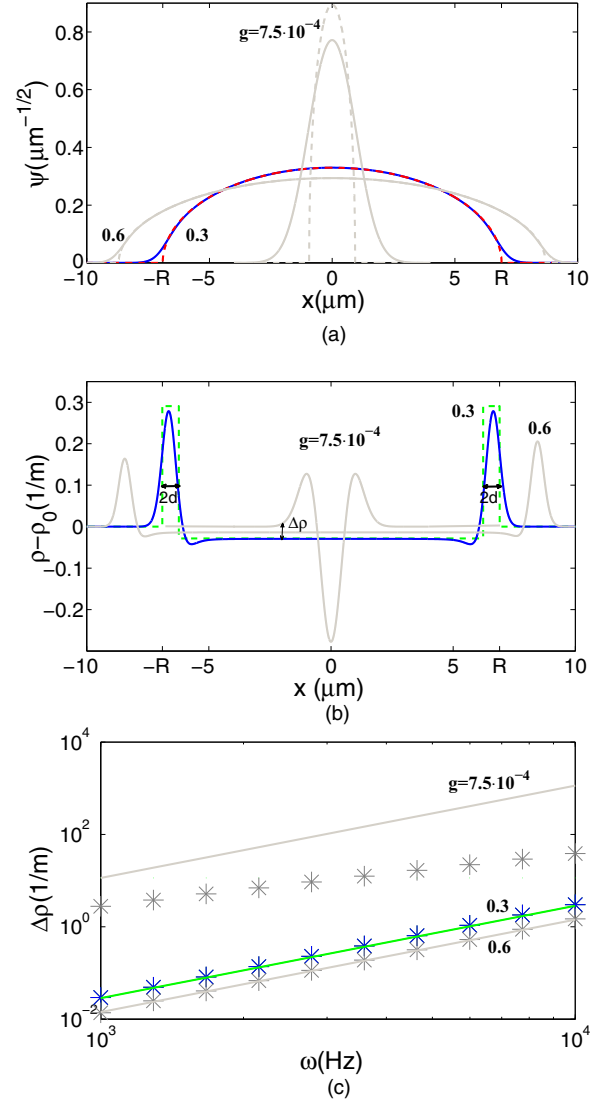


FIG. 1. (Color online) Ground state of rubidium atoms  $m = 87$  (amu) for various interaction parameters  $g$  marked in the figure. The results for  $g = 0.3$  (Hz m) are colored while the ones for stronger or weaker nonlinearities are marked by light gray. If  $g$  is too small, the TF approximation is not valid and there is a big difference between the theory and the numerical results. (a) Ground-state wave function of the GPE calculated with the help of (37) (solid line) and the Thomas-Fermi approximation (31) or (32) (dashed line) for  $\omega = 1$  (kHz). (b) Solid line: Calculated density deviations [using (37)] due to nonzero van der Waals radius  $\rho[l = 5$  (nm)]  $-\rho_0(l = 0)$ ,  $\omega = 1$  (kHz). Dashed green line: simple approximation (B3) for the deviations. Here  $d = 0.3$  ( $\mu\text{m}$ ) [for  $g = 0.3$  (Hz m)], as can be found from (20) and (34). Note that the deviations between the TF results and the GP ones as well as between  $\rho$  and  $\rho_0$  are largest in a region of size  $d$  around  $x = R$ . The deviations for  $g = 7.5 \times 10^{-4}$  (Hz m) are divided by 10 in order to make the figure clear. (c) Density deviations at the center  $x = 0$  of the trap  $\Delta\rho = \rho_0(l = 0) - \rho[l = 5$  (nm)] as a function of the trapping frequency  $\omega$ . The solid line is the prediction (35) and the stars are the numerically calculated values using (37). The scale is logarithmic.

where we expand  $\Delta E$  in powers of  $\delta\rho$  with constants  $C_0^{\text{pert}}$  and  $C_1^{\text{pert}}$  [see (B24) and (B21) in Appendix B]. This minimum is

obtained for

$$\delta\rho = \Delta\rho = -\frac{C_1^{\text{pert}}}{2C_2^{\text{GP}}} \quad (45)$$

and the resulting value of  $E$  is

$$E = E(l=0) - \frac{(C_1^{\text{pert}})^2}{2C_2^{\text{GP}}} + C_0^{\text{pert}}(l). \quad (46)$$

The parameters  $C_2^{\text{GP}}$ ,  $C_1^{\text{pert}}$ , and  $C_0^{\text{pert}}(l)$  are calculated explicitly in Appendix B [Eqs. (B11), (B21), and (B24)]. From (40) we see that  $C_0^{\text{pert}}(l)$  and  $C_1^{\text{pert}}(l)$  are proportional to  $l^2$ . Therefore in the leading order  $\frac{C_1^{\text{pert}}(l)^2}{2C_2^{\text{GP}}}$  can be neglected. The leading-order correction to the energy which is related to the van der Waals radius is [see (B24)]

$$\Delta E_0(l) \approx C_0^{\text{pert}} = -\frac{g}{4} \int_{-R}^R l^2 \frac{d^2 \rho_0(x)}{dr^2} \rho_0(x) dx. \quad (47)$$

and using (32) we obtain in the leading order in  $l^2$

$$\Delta E(l) \approx \frac{1}{4} m l^2 \omega^2. \quad (48)$$

This is the main result of the present work. Since the correction to the chemical potential given by (36) turns out not to depend on the density, we obtain the same correction for the energy per particle (48). The correction (48) is very small compared to the total energy (27),

$$\frac{\Delta E(l)}{E(l=0)} = \frac{5l^2}{12} \left( \frac{2^{5/2} m \omega^2}{3g} \right)^{2/3} = \frac{5}{6} \frac{l^2}{R^2} = -\frac{5}{3} \frac{g_2}{R^2}, \quad (49)$$

where  $R$  is given by (20). Although the correction (48) is small for realistic parameters, we believe that it can be measured because it is linear in  $\omega^2$  while  $E(l=0) \propto \omega^{2/3}$  (27) (see Fig 2). In the discussion (Sec. V), we present estimates for the magnitude of the correction (48). In particular, a possibility to substantially increase  $l$  with the help of Feshbach resonances is discussed. Furthermore, using molecules [13,14] or Rydberg atoms [15] instead of atoms in their ground state is likely to increase significantly the length  $l$  and hence to increase  $\Delta E(l)$ . From Fig. 2(b), it is seen that in the TF regime, the correction to the energy does not depend on  $g$  [and therefore the lines for  $g = 0.3$  (Hz m) and  $g = 0.6$  (Hz m) merge], while for weaker nonlinearity parameters the correction does depend on  $g$  and disagrees with our theoretical results.

## V. SUMMARY AND DISCUSSION

In this work we introduce a simple model (5) taking into account the extension of interparticle potential, and calculate the corrections to the standard GPE where  $\delta$ -function interaction potentials are assumed. For realistic experimental parameters we find that these corrections are indeed small. We calculate the correction for a Bose-Einstein condensate in a harmonic trap, in a situation where in most of the volume of the trap the Thomas Fermi (TF) approximation is valid. The correction to the ground-state energy is given in the leading order by (48), namely,

$$\Delta E(l) = \frac{1}{4} m l^2 \omega^2, \quad (50)$$

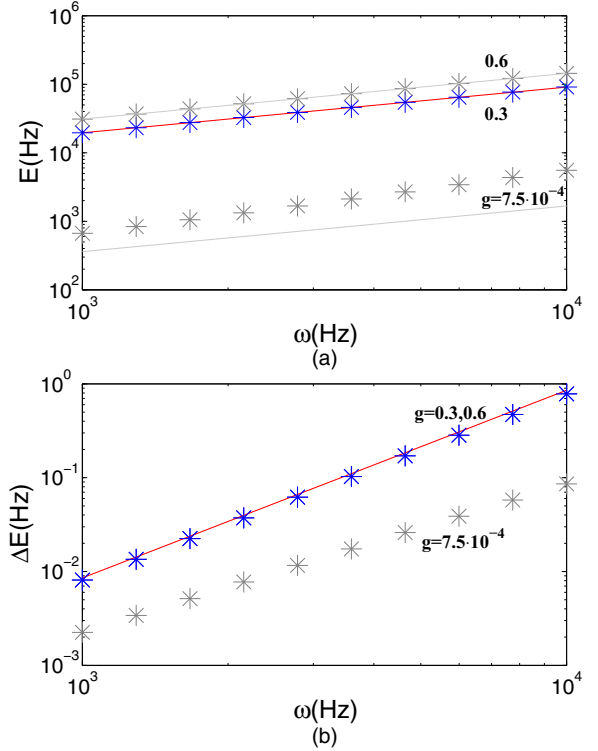


FIG. 2. (Color online) Energy of the ground state of rubidium BEC as a function of the trap frequency  $\omega$  for various interaction parameters  $g$  marked in the figure. The results for  $g = 0.3$  (Hz m) are colored while the ones for stronger or weaker nonlinearities are marked by light gray. (a) Energy for  $l = 0$ . solid line: the prediction (27); stars: the calculated values integrating (37). (b) The correction to the energy  $\Delta E(l) = E[l = 5 \text{ (nm)}] - E[l = 0]$ . Solid red line: the prediction (48); stars: the calculated values integrating (37).

where  $m$  is the mass of the particles,  $l$  is the extension of the potential (related to the van der Waals radius), and  $\omega$  is the frequency of the confining harmonic trap. By setting  $l$  equal to the typical range of van der Waals potentials (about  $100a_0$  where  $a_0 = 0.5 \text{ \AA}$  is the Bohr radius) and using a small condensate of size of  $R = 10 \text{ \mu m} \approx 2 \times 10^5 a_0$ , we find a relative correction [Eq. (49)] of  $10^{-6}$  which is extremely small and hard to measure. However, as discussed in Ref. [16] (see also [17,18]), the effective range diverges near Feshbach resonances and zero crossings of the scattering length. In particular, near zero crossing [12],

$$g_2 \sim -\frac{r_{e0} a_{bg}^2}{2a}, \quad (51)$$

where the relevant length scales are  $r_{e0}$  (the effective range at the Feshbach resonance),  $a_{bg}$  (the background scattering length), and  $a$  (the scattering length). For a broad resonance, the effective range is larger than the van der Waals radius, for a narrow resonance, it can be much larger [5]. Assuming both  $r_{e0}$  and  $a_{bg}$  are of the order of the van der Waals radius, namely  $100a_0$ , we estimate

$$g_2 \approx -10^6 \frac{a_0^3}{2a}. \quad (52)$$



Zero crossings of scattering lengths have been resolved to within  $0.01a_0$  [19]. Assuming  $a \approx 0.1a_0$ , we obtain a  $g_2$  of  $\approx -10^7 a_0^2$ . Taking  $R = 10$  ( $\mu\text{m}$ ) implies a relative energy correction (49) due to the finite extension of the potential of the order of  $\frac{1}{2} \times 10^{-3}$ , which could be even larger for smaller condensates (using for example atom chips with tight confinement) and atoms with larger background scattering lengths or narrow Feshbach resonances. The TF approximation is still valid since for sufficiently high atom number  $N$ , the TF radius  $R$  [Eq. (20)],

$$R = \left( \frac{3}{2m} g \omega^{-2} \right)^{1/3} = a_{\parallel} \left( \frac{3Naa_{\parallel}}{a_{\perp}^2} \right)^{1/3}, \quad (53)$$

can always be made larger than the oscillator length  $a_{\parallel}$ . Here  $a_{\parallel} = \sqrt{\frac{\hbar}{m\omega}}$  and  $a_{\perp} = \sqrt{\frac{\hbar}{m\omega_{\perp}}}$  are the harmonic trap length scales in the parallel ( $x$ ) and the transverse ( $y, z$ ) directions respectively. For the scattering length of  $0.1a_0$  assumed above,  $a_{\parallel}$  of the order of 2 ( $\mu\text{m}$ ) and  $a_{\perp} \approx 0.2$  ( $\mu\text{m}$ ), an atom number of  $N > 10^5$  ensures the validity of the TF approximation.

Our results apply also to novel condensates of molecules [13,14,20], photons [21], and polaritons [22,23] where the correction to the GPE may be larger. There are other corrections to the GPE, for example, the Lee-Yang-Huang (LYH) correction [1] which is typically larger than the correction that was considered here and is fundamentally of a different origin, as it depends on the density of particles while the correction (50) does not depend on this quantity. These corrections scale differently with the trap frequency  $\omega$ . In elongated traps, the LYH correction is linear in  $\omega$  and can in principle be distinguished from the correction calculated here which is proportional to  $\omega^2$ . Our calculations are in one dimension, but the extension to higher dimensions is straightforward.

The approach of capturing the physics of realistic potentials by several  $\delta$  functions should have many applications beyond the purpose of this paper.

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#### APPENDIX A

In this Appendix, we calculate the phase shift for the “ $\delta$  atom” (5), which can be used for defining the one-dimensional toy model (11) and determining  $\frac{1}{2}J^2$  in Eq. (12).

The characteristic length scales of the interactions are small compared to the length scales of the trapping potential and therefore we are allowed to assume that the external potential is constant over the interaction regime, i.e., the wave function  $\psi$  depends only on the relative distance  $r$  between two particles

and out of the pair interaction range, the particles are assumed to be free. In the absence of interactions, the wave function is a free wave

$$\psi(r) = A \frac{\sin(kr)}{r}, \quad (A1)$$

where  $k = \sqrt{2mE/\hbar^2}$ . Interactions will add a phase shift  $\delta$ , so that for  $r > r_{\text{out}}$ ,

$$\psi(r) = A \frac{\sin(kr + \delta)}{r}. \quad (A2)$$

We turn now to calculate  $\delta$ , the phase shift caused by the potential (5). In Ref. [6], it is argued that the phase shift is related to the pair interaction energy  $E_{\text{pair}}$  [Eq. (6) of [6]] by

$$E_{\text{pair}} = \frac{2\hbar^2 k}{m} \left( -\frac{\delta}{L} \right). \quad (A3)$$

Here, the nonlinear energy of each particle is

$$E_{nl} = N E_{\text{pair}}, \quad (A4)$$

where  $E_{nl}$  is the change in the energy that the scattering potential could cause if the particles were constrained to stay in a large ball of radius  $L$  while  $E_{\text{pair}}$  is the interaction energy of a single pair of particles. The energy shift  $E_{\text{pair}}$  is calculated using perturbation theory of the lowest order in  $r_{\text{in}}$ ,  $\lambda$ , and  $g_{3D}$ :

$$\begin{aligned} E_{\text{pair}} &\approx \int_0^{r_{\text{in}}} 4\pi r^2 |\psi(r)|^2 \frac{3(g_{3D} + \lambda)}{4\pi r_{\text{in}}^3} dr \\ &\quad - \int_0^{\infty} 4\pi r^2 |\psi(r)|^2 \frac{\lambda}{4\pi r_{\text{out}}^2} \delta(r - r_{\text{out}}) dr \\ &= \frac{3(g_{3D} + \lambda)}{r_{\text{in}}^3} \int_0^{r_{\text{in}}} r^2 |\psi(r)|^2 dr - \lambda |\psi(r_{\text{out}})|^2. \end{aligned} \quad (A5)$$

Using  $\psi(r)$  of (A2), and in the limit  $r_{\text{in}} \rightarrow 0$  one finds

$$E_{\text{pair}} \approx A^2 \left[ (g_{3D} + \lambda) k^2 - \lambda \frac{\sin^2(kr_{\text{out}})}{r_{\text{out}}^2} \right]. \quad (A6)$$

The normalization constant  $A$  should satisfy

$$A^2 \int_0^L 4\pi \sin^2(kr) dr = 1. \quad (A7)$$

Remembering that  $L$  is very large,

$$\begin{aligned} \int_0^L \sin^2(kr) dr &= \frac{1}{2} \int_0^L [1 - \cos(2kr)] dr \\ &= \frac{L}{2} - \frac{1}{2k} \sin(2kL) \approx \frac{L}{2} \end{aligned} \quad (A8)$$

and therefore  $A = 1/\sqrt{2\pi L}$ . Combining (A3) and (A6), we end up with

$$\begin{aligned} \delta &= -\frac{LmE_{\text{pair}}}{2\hbar^2 k} \\ &= -\frac{m}{4\pi\hbar^2 k} \left[ (g_{3D} + \lambda) k^2 - \lambda \frac{\sin^2(kr_{\text{out}})}{r_{\text{out}}^2} \right] \\ &\approx \frac{m}{4\pi\hbar^2} \left[ -(g_{3D} + \lambda) k + \lambda \left( k - \frac{2}{3} r_{\text{out}}^2 k^3 \right) \right]. \end{aligned} \quad (A9)$$

Here we used the fact that the wavelength is large. This leads to a total phase shift of

$$\delta = -\frac{g_{3D}m}{4\pi\hbar^2}k - \frac{m}{4\pi\hbar^2}\frac{2}{3}r_{\text{out}}^2\lambda k^3. \quad (\text{A10})$$

In order to calculate the scattering length and the effective range, we write  $k \cot(\delta)$  as a power series in  $k$ :

$$k \cot(\delta) = -\frac{1}{a} + \frac{1}{2}r_e k^2. \quad (\text{A11})$$

Define  $C_3 \equiv -\frac{m\lambda}{4\pi\hbar^2}\frac{2}{3}r_{\text{out}}^2$  so that  $\delta = -ak + C_3k^3$  and

$$k \cot(\delta) = \frac{k}{\tan(\delta)} \approx \frac{k}{\delta} \left(1 - \frac{1}{3}\delta^2\right), \quad (\text{A12})$$

where it is assumed that  $\delta \ll 2\pi$ . The expansion in a power series of  $k$  yields

$$\begin{aligned} k \cot(\delta) &\approx \frac{1}{-a + C_3k^2} \left(1 - \frac{1}{3}(-a + C_3k^2)^2k^2\right) \\ &\approx -\frac{1}{a} \left(1 + \frac{C_3}{a}k^2\right) \left(1 - \frac{1}{3}a^2k^2\right) \\ &\approx -\frac{1}{a} \left[1 + \left(\frac{C_3}{a} - \frac{1}{3}a^2\right)k^2\right]. \end{aligned} \quad (\text{A13})$$

According to (A11) and (A13),

$$r_e = -2 \left[ \frac{C_3}{a^2} - \frac{1}{3}a \right] \quad (\text{A14})$$

so that

$$g_2 = a \left( \frac{a}{3} - \frac{r_e}{2} \right) = \frac{C_3}{a} = -\frac{2\lambda}{3g_{3D}}r_{\text{out}}^2, \quad (\text{A15})$$

resulting in the identification of  $\Delta E_{\text{int}}$  of (6).

## APPENDIX B

In this Appendix we calculate explicitly quantities used in Secs. III and IV. It turns out that in the leading order, the correction to the energy (48) does not depend on either  $\Delta\rho$  or the coefficients  $C_2^{\text{GP}}$  and  $C_1^{\text{GP}}$  [to be defined in Eq. (B7)]. However, we would like to compute it and find the analytical justification for (35). Using a variational principle, we analytically calculate  $\Delta\rho$  which is the value of  $\delta\rho$  which minimizes (44) and obtain the result (35). The expansion (44) of the energy as a power series in  $\delta\rho$  takes into account the energy corrections  $\Delta E_p = E_p - E_p(l=0)$  and  $\Delta E_{nl} = E_{nl} - E_{nl}(l=0)$ , given by

$$\Delta E_p = \int [\rho(x) - \rho_0(x)] U(x) dx \quad (\text{B1})$$

and

$$\Delta E_{nl} = \frac{g}{2} \int dx \left\{ [\rho^2(x) - \rho_0^2(x)] - \frac{1}{2}l^2 \frac{d^2\rho(x)}{dx^2} \rho(x) \right\}. \quad (\text{B2})$$

In the regime where the Thomas-Fermi (TF) approximation is valid,  $-R \lesssim x \lesssim R$ , we showed [Eq. (33)] that for a harmonic potential,  $\rho(x) = \rho_0(x) - \delta\rho$ , where  $\delta\rho$  is small and does not depend on  $x$ . At  $x \approx \pm R$ ,  $\rho(x) - \rho_0(x)$  has sharp picks

with total integrated area of approximately  $2R\delta\rho$ . Thus, it is convenient to introduce a simplified density

$$\rho(x) = \begin{cases} \rho_0(x) - \delta\rho, & |x| < R - 2d, \\ \rho_0(x) + \frac{R}{2d}\delta\rho, & R - 2d < |x| < R \end{cases} \quad (\text{B3})$$

for calculating the energies. This density [dashed line in Fig. 1(b)] assumes that the correction resulting of the finite range of interaction is piecewise constant. It can be used to estimate integrals involving the density and smooth quantities. This approximate density was introduced since we know to calculate the density only in  $[0, R - 2d]$  where the TF approximation is valid. The estimate (B3) of  $\rho(x)$  in the interval  $[R - 2d, R]$  relies on the fact that both  $\rho$  and  $\rho_0$  are normalized to 1. Using the density (B3) and the relation (20) for calculating the deviation (B1), one finds (taking for each order of  $\delta\rho$  only the leading term in  $\frac{d}{R}$ , assumed to be small when the TF approximation is valid)

$$\begin{aligned} \Delta E_p &\approx \delta\rho \left[ -\int_{-R+2d}^{R-2d} U(x) dr + \frac{R}{d} \int_{R-2d}^R U(x) dr \right] \\ &= \delta\rho \left\{ -\frac{1}{3}m(R-2d)^3\omega^2 \right. \\ &\quad \left. + m\frac{R}{6d}[R^3 - (R-2d)^3]\omega^2 \right\} \\ &= mR^3\omega^2\delta\rho \left( \frac{2}{3} - \frac{8}{3}\frac{d^2}{R^2} + \frac{8}{3}\frac{d^3}{R^3} \right) \\ &\approx \frac{2}{3}mR^3\omega^2\delta\rho = g\delta\rho. \end{aligned} \quad (\text{B4})$$

The deviation (B2) can be divided in two parts

$$\Delta E_{nl} = \Delta E_{nl}^{\text{GP}} + \Delta E_{nl}^{\text{pert}}. \quad (\text{B5})$$

The first contribution to  $\Delta E_{nl}$ , caused only by the changes in the wave function, is

$$\begin{aligned} \Delta E_{nl}^{\text{GP}} &= \frac{g}{2} \int dx [\rho^2(x) - \rho_0^2(x)] \\ &\approx g \int_{-R+2d}^{R-2d} \left[ -\rho_0(x)\delta\rho + \frac{1}{2}\delta\rho^2 \right] dx \\ &\quad + 2g \int_{R-2d}^R \left[ \rho_0(x)\frac{R}{2d}\delta\rho + \frac{R^2}{8d^2}\delta\rho^2 \right] dx \end{aligned} \quad (\text{B6})$$

that can be written in the form

$$\Delta E_{nl}^{\text{GP}} = C_1^{\text{GP}}\delta\rho + C_2^{\text{GP}}\delta\rho^2, \quad (\text{B7})$$

and the second contribution, caused by the additional term in Eq. (B2), is

$$\begin{aligned} \Delta E_{nl}^{\text{pert}} &= -\frac{g}{4} \int l^2 \frac{d^2\rho(x)}{dx^2} \rho(x) dx \\ &\approx -\frac{g}{4} \int_{-R+2d}^{R-2d} l^2 \frac{d^2\rho_0(x)}{dx^2} [\rho_0(x) - \delta\rho] dx \\ &\quad - \frac{g}{2} \int_{R-2d}^R l^2 \frac{d^2\rho_0(x)}{dx^2} \left[ \rho_0(x) + \frac{R}{2d}\delta\rho \right] dx. \end{aligned} \quad (\text{B8})$$

that can be written in the form

$$\Delta E_{nl}^{\text{pert}} = C_0^{\text{pert}} + C_1^{\text{pert}}\delta\rho. \quad (\text{B9})$$

Remembering that  $\int_{-R+2d}^{R-2d} \rho_0(x) \approx 1$ , we get

$$C_1^{\text{GP}} = -g + \frac{Rg}{d} \int_{R-2d}^R \rho_0(x) dx, \quad (\text{B10})$$

$$C_2^{\text{GP}} = g(R-2d) + g \frac{R^2}{2d} \approx g \frac{R^2}{2d}, \quad (\text{B11})$$

$$C_0^{\text{pert}} = \frac{1}{4} ml^2 \omega^2 - \frac{g}{2} \int_{R-2d}^R l^2 \rho_0(x) \frac{d^2 \rho_0(x)}{dx^2} dx, \quad (\text{B12})$$

$$C_1^{\text{pert}} = -\frac{1}{4} ml^2 \omega^2 (2R-4d) - \frac{gR}{4d} l^2 \int_{R-2d}^R \frac{d^2 \rho_0(x)}{dx^2} dx. \quad (\text{B13})$$

We turn now to calculate the various terms assuming  $\frac{d}{R} \ll 1$  and begin by estimating the second term in Eq. (B10). Since  $\rho_0(x)$  decreases with  $x$  for  $x > 0$ ,

$$\begin{aligned} \frac{Rg}{d} \int_{R-2d}^R \rho_0(x) dx &\ll \frac{Rg}{d} 2d \rho_0(R-2d) \\ &= 2Rg \rho_0(R-2d). \end{aligned} \quad (\text{B14})$$

For  $\rho_0(R-2d)$  we can use the TF approximation (32) and (17):

$$\begin{aligned} 2Rg \rho_0(R-2d) &\approx 2R \left( \mu - \frac{1}{2} m \omega^2 (R^2 - 4Rd) \right) \\ &= 4R^2 m \omega^2 d = 8\mu d. \end{aligned} \quad (\text{B15})$$

Using (19) and (20) we see that

$$\mu R = \frac{3}{4} g \quad (\text{B16})$$

and therefore  $8\mu d = 6g \frac{d}{R}$  is much smaller than  $g$  taking into account  $d \ll R$ .

Hence, it is justified to estimate

$$C_1^{\text{GP}} \approx -g \quad (\text{B17})$$

as expected (since  $\delta\rho$  minimizes the energy for  $l=0$ , the sum of  $\Delta E_p$  and  $C_1^{\text{GP}} \delta\rho$  must vanish). Now we turn to estimate  $C_1^{\text{pert}}$ . In Eq. (B13), we have a term proportional to  $\int_{R-2d}^R \frac{d^2 \rho_0(x)}{dx^2} dx$ . We do not have an explicit expression for the function  $\rho_0$  in the interval  $[R-2d, R]$ , but since  $\frac{d\rho_0}{dx} \approx 0$  for  $x > R$ ,

$$0 = \int_0^{R-2d} \frac{d^2 \rho_0(x)}{dx^2} + \int_{R-2d}^R \frac{d^2 \rho_0(x)}{dx^2} dx. \quad (\text{B18})$$

In the interval  $[0, R-2d]$  the TF approximation results in Eq. (32), so,

$$\begin{aligned} \int_{R-2d}^R \frac{d^2 \rho_0(x)}{dx^2} dx &= - \int_0^{R-2d} \frac{d^2 \rho_0(x)}{dx^2} dx \\ &\approx \frac{(R-2d) m \omega^2}{g}. \end{aligned} \quad (\text{B19})$$

The coefficient  $C_1^{\text{pert}}$  (B13) is given by

$$\begin{aligned} C_1^{\text{pert}} &= -\frac{1}{4} ml^2 \omega^2 (2R-4d) - \frac{gR}{4d} l^2 \int_{R-2d}^R \frac{d^2 \rho_0(x)}{dx^2} dx \\ &\approx -\frac{1}{4} ml^2 \omega^2 (2R-4d) - \frac{R}{4d} l^2 (R-2d) m \omega^2 \end{aligned} \quad (\text{B20})$$

and the leading order in  $\frac{d}{R}$  is

$$C_1^{\text{pert}} = -\frac{R^2}{4d} l^2 m \omega^2. \quad (\text{B21})$$

We calculate now  $C_0^{\text{pert}}$ . Equation (B12) contains an integral of the form

$$\begin{aligned} l^2 g \int_{R-2d}^R \rho_0(x) \frac{d^2 \rho_0(x)}{dx^2} dx \\ \ll l^2 g \rho_0(R-2d) \int_{R-2d}^R \frac{d^2 \rho_0(x)}{dx^2} dx. \end{aligned} \quad (\text{B22})$$

The integral over the second derivative of  $\rho_0$  was already calculated in Eq. (B19) and we can estimate

$$l^2 g \int_{R-2d}^R \rho_0(x) \frac{d^2 \rho_0(x)}{dx^2} dx \ll (R-2d) m \omega^2 l^2 \rho_0(R-2d). \quad (\text{B23})$$

Using (B15) and (B16), it turns out that the second term in Eq. (B12) is negligible, hence,

$$C_0^{\text{pert}} \approx \frac{1}{4} ml^2 \omega^2. \quad (\text{B24})$$

Now, it is possible to calculate  $\Delta\rho$ . Let us write the ground state of the standard GPE as a minimum with respect to  $\delta\rho$  of

$$E^{\text{GP}}(\delta\rho) \approx E^{\text{GP}}(0) + \Delta E_p^{\text{GP}} + \Delta E_{nl}^{\text{GP}}. \quad (\text{B25})$$

Using the previous results (B4), (B7), (B11), and (B17) we end up with

$$E^{\text{GP}}(\delta\rho) = E^{\text{GP}}(0) + \frac{gR^2}{2d} \delta\rho^2. \quad (\text{B26})$$

If we repeat this calculation for the modified GPE (12), we should add the term (B9) to (B26). According to (B21) and (B24),

$$\Delta E_{nl}^{\text{pert}} = \frac{1}{4} ml^2 \omega^2 - \frac{R^2}{4d} l^2 m \omega^2 \delta\rho. \quad (\text{B27})$$

The resulting equation for the energy is

$$E(\delta\rho) = E^{\text{GP}}(0) + \frac{1}{4} ml^2 \omega^2 - \frac{R^2}{4d} l^2 m \omega^2 \delta\rho + \frac{gR^2}{2d} (\delta\rho)^2. \quad (\text{B28})$$

The minimum is found for

$$\delta\rho = \Delta\rho = -\frac{-\frac{1}{4d} l^2 m \omega^2 R^2}{2\left(\frac{gR^2}{2d}\right)} = \frac{1}{4g} l^2 m \omega^2. \quad (\text{B29})$$

This result is in agreement with (35) found numerically.

The energy of the modified GPE for  $\delta\rho = \Delta\rho$  is

$$\begin{aligned} E(\Delta\rho) &= E^{\text{GP}}(0) + \frac{gR^2}{2d} \Delta\rho^2 + \frac{1}{4} ml^2 \omega^2 - \frac{R^2}{4d} l^2 m \omega^2 \Delta\rho \\ &= E^{\text{GP}}(0) + \frac{1}{4} ml^2 \omega^2 - \frac{1}{32g} l^4 m^2 \omega^4, \end{aligned} \quad (\text{B30})$$

which agrees (in first order in  $l^2$ ) with (48).



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