J Math Chem (2010) 47:636–646
DOI 10.1007/s10910-009-9591-8

ORIGINAL PAPER

The effect of the negative coupling parameter on the spectrum of a trapped Bose gas

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Received: 13 January 2009 / Accepted: 17 August 2009 / Published online: 4 September 2009

Abstract The interest in attractive Bose–Einstein Condensates arises due to the chemical instabilities generate when the number of trapped atoms is above a critical number. In this case, recombination process promotes the collapse of the cloud. This behavior is normally geometry dependent. Within the context of the mean field approximation, the system is described by the Gross–Pitaevskii equation. We have considered the attractive Bose–Einstein condensate, confined in a nonspherical trap, investigating numerically and analytically the solutions, using controlled perturbation and self-similar approximation methods. This approximation is valid in all interval of the negative coupling parameter allowing interpolation between weak-coupling and strong-coupling limits. When using the self-similar approximation methods, accurate analytical formulas were derived. These obtained expressions are discussed for several different traps and may contribute to the understanding of experimental observations.

Keywords Bose–Einstein condensation · Negative coupling parameter

1 Introduction

Cold atomic interactions occupy a strategic position, contributing for many fields involved in chemical physics, atomic and molecular physics and even in condensed matter. Being in the intersection of many subjects, it presents a wide interest and

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a tremendous growth of interest. For many years, a great deal of research was devoted to the field of cold collisions [1]. With the advent of controlled Bose-Condensation, the interest moves many orders of magnitude down in temperature, reaching the domain where a full quantum description is necessary. In that case, a renewing interest of the chemistry of ultra-low temperatures experienced a revival. During the occurrence of Bose–Einstein condensation, the dissipative process like three body recombination, are dominated by the sign of the effective interaction represented by the magnitude and sign of the quantity "scattering length". In the presence of interaction, a confined collection of bosons that undergo Bose-Condensation has many of the properties modified. The peculiar properties associated with the occurrence of Bose-condensation revels many unresolved mathematical problems and renewed flurry of interest in those questions. The subject is largely quiescent due to the developing of experiments that provides feedback for theories and approximations. Among the topics of interest is the case of Bose–Einstein condensation of trapped atomic gases with attractive interactions. The system is normally described by the Gross–Pitaevskii Equation (GPE) [2–4] and was realized in ultracold vapors of ^{7}Li by Bradley et al. [5], opening a new field in the study of macroscopic quantum phenomena. The interest in this case arises due to the chemical instability associated with the negative interaction in the quantum cloud of atoms. The knowledge of the spectrum of the trapped cloud is, in this case, fundamental to understand the spatial distribution and the macroscopic behavior associated with collapse of the condensate. Within the mean field approximation, the system presents modification of the overall allowed energies of the occupying potential. In describing the system within the GPE, there is a competition involving the nonlinear term due to the contact interaction and the remaining energy terms. This competition, for the case of negative scattering length, is what determines the observed instabilities. The overall behavior of those instabilities is sensitive to the spatial distribution of the cloud, and therefore is dependent on the trap geometry, generating interest for the possible calculation of the gas spectrum in different geometries of atomic traps. The nonlinear GPE has no exact solution and for practical applications one needs to resort to some approximations, for example: the Gaussian and Thomas-Fermi approximations. The mathematical structure of the GPE is of nonlinear Schrödinger equation. The stationary states, due to the confinement caused by trapping potential, possess discrete energy levels. These stationary eigenstates form a set of solutions that can be called nonlinear coherent modes, analogue to linear modes that are solutions of a linear Schrödinger equation. So, the wave function of the GPE corresponds to a coherent state of Bose condensed atoms. The properties of these modes have been calculated theoretically in several publications [6–11] and a nonlinear dipole mode was observed experimentally [12]. In particular interest is the comparison of precision when different methods are employed in the evaluation of the GPE equation for specific geometries.

The aim of the present paper is to calculate a numerical approximate solution to the GPE with cylindrical symmetry and an analytical approximate solution to this same equation, such that the coupling parameter has negative value, since the positive coupling parameter has been already solved by Yukalov [13–15]. Here we will yield asymptotically exact solutions in both limits of weak as well as strong coupling using negative values of the coupling parameter.

2 Cylindrical model

Atomic interactions for dilute trapped gases are well described by the Fermi contact potential because the ultra low energies make the interaction shape independent. The interatomic potential is therefore given by:

$$\Phi(r) = A\delta(r), \quad A \equiv 4\pi\hbar^2 \frac{a_s}{m_0}, \tag{1}$$

where a_s is the s-wave scattering length, m_0 is the atomic mass and A is the interaction parameter for the external confining potential. When we consider a harmonic trap as

$$U(r) = \frac{m_0}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right), \tag{2}$$

the quantum description of the trapped atoms is in the GPE, which for a system of N particles can be written as

$$\hat{\mathrm{H}}(\varphi) = -\frac{\hbar^2\nabla^2}{2m_0} + U(r) + NA\,|\varphi|^2, \tag{3}$$

where A is the interaction parameter and $U(r)$ the confining potential.

Here we shall consider a harmonic potential of cylindrical symmetry with radial frequency

$$\omega_r \equiv \omega_x = \omega_y$$

and axial frequency, ω_z, such that the anisotropy parameter, λ, and oscillator length, l_r, are defined as

$$\lambda \equiv \frac{\omega_z}{\omega_r}, \quad l_r \equiv \sqrt{\frac{\hbar}{m_0\omega_r}}. \tag{4}$$

The coupling parameter is defined as

$$g \equiv 4\pi \frac{a_s}{l_r} N \tag{5}$$

The nonlinear eigenproblem for the Hamiltonian of Eq. 3 cannot be solved exactly. The standard perturbation theory starting with a harmonic-oscillator approximation cannot be employed if arbitrary amplitude of the coupling parameter defined in Eq. 5 is considered. It is possible to find accurate approximate expressions for the whole spectrum for arbitrary values of the coupling parameter by means of the controlled perturbation theory [16–19].

3 Cylindric confining potential

To calculate the spectrum of the equation $\hat{\mathrm{H}}\,\Psi_n = E_n\Psi_n$ we may employ the controlled perturbation theory [20], and we can start with the initial Hamiltonian of a harmonic oscillator

$$\hat{\mathrm{H}}_0 = -\frac{1}{2}\nabla^2 + \frac{1}{2}\left(u^2r^2 + v^2z^2\right) \tag{6}$$

having two trial parameters, u and v [15]. Then, the eigenvalues of the operator in Eq. 6 are determined through

$$E^{(0)}_{nmk} = (2n + |m| + 1)\,u + \left(k + \frac{1}{2}\right)v, \tag{7}$$

where the radial quantum number $n = 0, 1, 2, \ldots$, the azimuthal number $m = 0, \pm1, \pm2, \ldots$, and the axial quantum number $k = 0, 1, 2, \ldots$. The corresponding eigenfunctions are

$$\Psi^{(0)}_{nmk}(r, \varphi, z) = \left[\frac{2n!u^{|m|+1}}{(n + |m|)!}\right]^{1/2} r^{|m|} \exp\left(-\frac{1}{2}ur^2\right) L^{|m|}_n\left(ur^2\right) \times \frac{e^{im\varphi}}{\sqrt{2\pi}} \frac{(v/\pi)^{1/4}}{\sqrt{2^k k!}} \exp\left(-\frac{1}{2}vz^2\right) \mathrm{H}_k\left(\sqrt{v}z\right)$$

where $L^m_n(\cdot)$ are the Laguerre polynomials and $\mathrm{H}_k(\cdot)$ are a Hermite polynomial.

In first order, we have

$$E^{(1)}_{nmk}(g, u, v) = \left(\Psi^{(0)}_{nmk}, \hat{\mathrm{H}}\,\Psi^{(0)}_{nmk}\right). \tag{8}$$

To write down this integral explicitly, it is convenient to use the notation

$$I_{nmk} \equiv \frac{1}{u\sqrt{v}} \int \left|\Psi^{(0)}_{nmk}(\vec{r})\right|^4 \mathrm{d}\vec{r}.$$

We can also introduce the follow combinations

$$p \equiv 2n + |m| + 1, \quad q \equiv 2k + 1. \tag{9}$$

Then, using the Rayleigh-Schrödinger perturbation theory, we may find a sequence $\{\mathrm{E}_k(g, u, v)\}$ of approximation orders $k = 0, 1, 2, \ldots,$ for the spectrum.

This way, the energy levels in Eq. 8 can be written as

$$E^{(1)}(g,u,v)=\frac{p}{2}\left(u+\frac{1}{u}\right)+\frac{q}{4}\left(v+\frac{\lambda^2}{v}\right)-\frac{1}{2}\frac{su\sqrt{\lambda}}{vp\sqrt{q}}. \tag{10}$$

The fixed-point conditions are, therefore, obtained from the conditions

$$\frac{\partial}{\partial u}E^{(1)}(g,u,v)=0,\quad \frac{\partial}{\partial v}E^{(1)}(g,u,v)=0. \tag{11}$$

Using Eq. 10 one will have

$$p\left(1-\frac{1}{u^2}\right)-\frac{s}{p\lambda}\sqrt{\frac{v}{q}}=0 \quad\text{and}\quad q\left(1-\frac{\lambda^2}{v^2}\right)-\frac{s}{p\lambda\sqrt{\lambda q}}=0 \tag{12}$$

for the control frequencies $u=u(g)$ and $v=v(g)$, where the notation

$$s\equiv -2p\sqrt{q}I_{nmk}\lambda g \tag{13}$$

is used. Substituting these control functions into Eq. 10, we obtain the controlled approximant

$$E(s)\equiv E^{(1)}[g(s),u(s),v(s)]. \tag{14}$$

Now, we can analyze the weak-coupling and strong-coupling limits in detail. In the weak-coupling limit (s very small), Eq. 12 gives the radial control function

$$\begin{aligned}u(s)\approx{}&-1-\frac{s}{2\sqrt{q\lambda}p^2}+\frac{s^2}{8q^2\lambda^2p^3}-\frac{3s^2}{8q\lambda p^4}+\frac{s^3}{4q^2\lambda^2\sqrt{-q\lambda}p^5}\\&+\frac{5s^3}{16q\lambda\sqrt{-q\lambda}p^6}+\frac{3s^3}{64q^3\lambda^3\sqrt{-q\lambda}p^4}\end{aligned} \tag{15}$$

and, respectively, the axial control function

$$\begin{aligned}v(s)\approx{}&\lambda-\frac{s}{2pq\sqrt{-q\lambda}}+\frac{s^2}{4q^3\lambda^2p^2}+\frac{s^2}{4q^2\lambda p^3}-\frac{3s^3}{16q^2\lambda p^5\sqrt{-q\lambda}}\\&+\frac{5s^3}{16q^3\lambda^2p^4\sqrt{-q\lambda}}-\frac{7s^3}{64q^4\lambda^3p^3\sqrt{-q\lambda}}\end{aligned} \tag{16}$$

In the strong-coupling limit (s very large), the radial control function is

$$u(s)\approx ps^{-2/5}+\frac{p\left(\lambda^2q^2-3p^2\right)}{5}s^{-6/5}-\frac{p\left(-\lambda^4q^4-\lambda^2q^2p^2+3p^4\right)}{5}s^{-2} \tag{17}$$

and for the axial control function we get

$$
v(s) \approx \lambda^2 q s^{-2/5} + \left(\frac{-4q\lambda^2 \left(+\lambda^2 q^2 - 3p^2\right)}{5} - 2p^2 q \lambda^2 \right) s^{-6/5}
+ \left(\begin{array}{l} p^4 q \lambda^2 \left(\frac{2\left(\frac{2\left(+6\lambda^4 q^4 - \lambda^2 q^2 p^2 - 6p^4\right)}{25p^2} + \frac{\left(+\lambda^2 q^2 - 3p^2\right)^2}{25p^2} \right)}{p^2} + \frac{4\left(+\lambda^2 q^2 - 3p^2\right)^2}{25p^4} \right) \\ +q\lambda^2 \left(p^4 + \frac{4p^2\left(+\lambda^2 q^2 - 3p^2\right)}{5} \right) + \frac{8p^2 q \lambda^2 \left(-\lambda^2 q^2 + 3p^2\right)}{5} \end{array} \right) s^{-2} \tag{18}
$$

Finally, for the weak-coupling limit, the energy in Eq. 14 becomes

$$
\mathrm{E}(s) \approx \left(-p + \frac{1}{2} q \lambda \right) + \frac{1}{2\sqrt{\lambda} p \sqrt{q}} s
+ \left(\begin{array}{l} -\frac{1}{8p^3 q \lambda} + \frac{1}{4} q \left(\begin{array}{l} \frac{1}{4q^3 \lambda^2 p^2} \\ + \frac{-\lambda\left(\frac{1}{4q^3\lambda^2 p^2} - \frac{1}{4q^2 \lambda p^3} \right) + \frac{1}{4p^2 q^3 \lambda}}{\lambda} - \frac{1}{4q^2 \lambda p^3} \end{array} \right) \\ - \frac{-\frac{2}{\lambda^{3/2} p q^{3/2}} + \frac{4\sqrt{\lambda}}{\sqrt{q\lambda} p^2}}{16 \lambda p \sqrt{q}} \end{array} \right) s^2 \tag{19}
$$

and for the strong-coupling limit we find

$$
E(s) \approx \left(\frac{3}{4} - \frac{\sqrt{q\lambda^2}}{2\lambda\sqrt{q}} \right) s^{2/5} + \left(\frac{p^2}{2} + \frac{q^2\lambda^2}{4} \right) s^{-2/5}. \tag{20}
$$

In the limit $s \rightarrow -\infty$ [20], we obtain the energy

$$
\mathrm{E}(s) \approx \frac{-\frac{3(-1)^{3/5}}{4} + \frac{(-1)^{2/5}\sqrt{\lambda^2 q (-1)^{2/5}}}{2\lambda\sqrt{q}}}{\left(-\frac{1}{s}\right)^{2/5}} + \left(\frac{p^2 (-1)^{2/5}}{2} + \frac{\lambda^2 q^2 (-1)^{2/5}}{4} \right) - s^{2/5} \tag{21}
$$

4 Cylindrical traps

Now we calculate the root approximants using the negative value of the effective interaction strength in Eq. 13, interpolating the weak-coupling in Eq. 19 and the strong-coupling in Eq. 20 of the spectrum and then we employ the self-similar approximation method, which was developed by Yukalov [21], and obtain

$$
\mathrm{E}^*_k(s) = a_0 \left(\left(\cdots (1 + A_{k1} s)^{n_{k1}} + A_{k2} s^2 \right)^{n_{k2}} + \cdots A_{kk} s^k \right)^{n_{kk}}. \tag{22}
$$

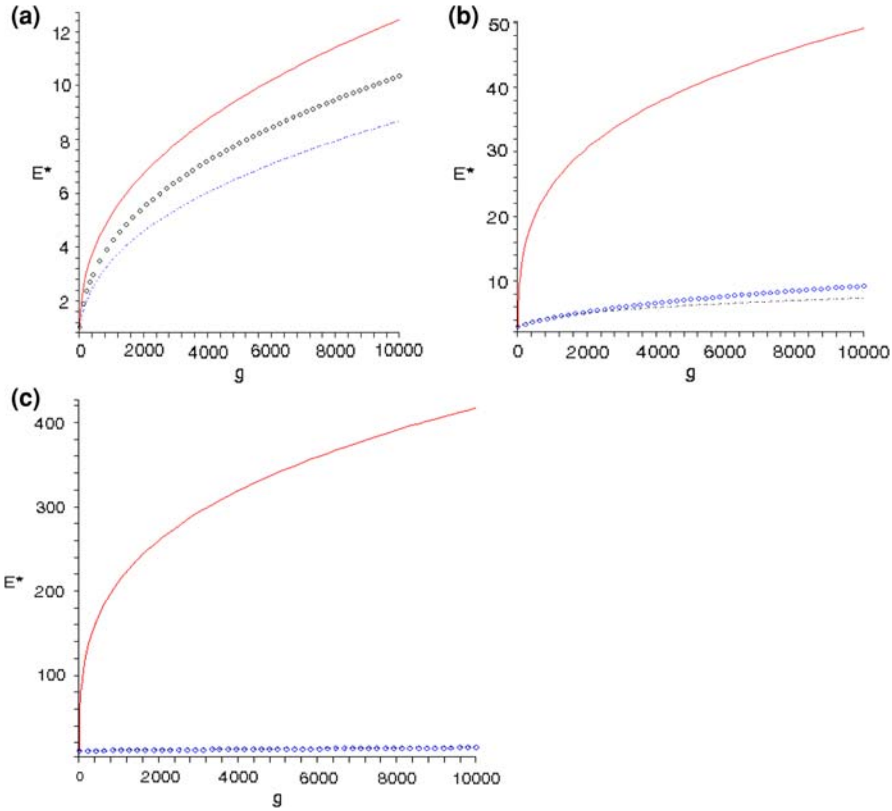

Fig. 1 Percentage errors of the self-similar approximants as functions of the coupling parameter g, in a cigar-shape trap, with $\lambda = 0.1$. E_1^* (*solid line*), E_2^* (*point line*), and E_3^* (*patch line*) are related with different quantum numbers: **a** $n = m = k = 0$; **b** $n = k = 0$, $m = 2$; **c** $n = k = 0$, $m = 10$

Depending on the approximation order $k = 1, 2, \ldots,$ in the first order, we have

$$E_1^*(s) = a_0 \,(1 + As)^{2/5} \tag{23}$$

where

$$a_0 = \left(-p + \frac{1}{2} q\lambda\right), \quad A^{2/5} = \frac{0.25}{a_0}.$$

In the second order

$$E_2^*(s) = a_0 \left[(1 + A_1 s)^{6/5} + A_2 s^2\right]^{1/5} \tag{24}$$

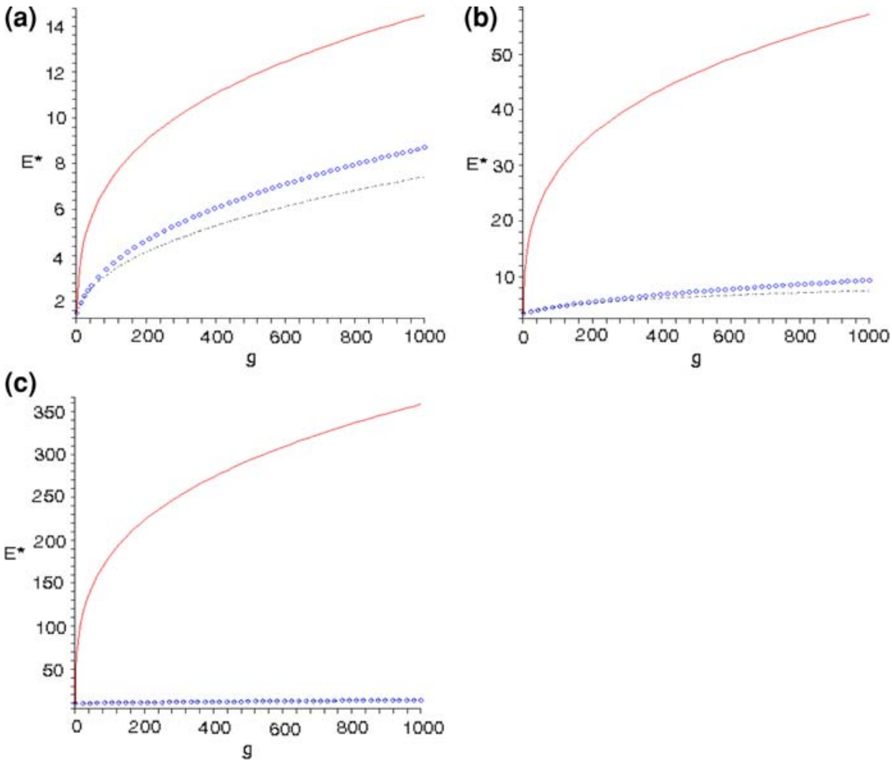

Fig. 2 Percentage errors of the self-similar approximants as functions of the coupling parameter g, in a spherical-shape trap, with $\lambda = 1$. E_1^* (*solid line*), E_2^* (*point line*), and E_3^* (*patch line*) are related with different quantum numbers: **a** $n = m = k = 0$; **b** $n = k = 0$, $m = 2$; **c** $n = k = 0$, $m = 10$

with same a_0 and with

$$A_1 = \frac{(0.25)^{25/6}}{a_0^{25/6}} \left[20 \left(\frac{p^2}{2} + \frac{(q\lambda)^2}{4} \right) \right]^{5/6}, \quad A_2^{1/5} = \frac{0.25}{a_0}.$$

In the third order we obtain

$$E_3^*(s) = a_0 \left\{ \left[(1 + B_1)^{6/5} + B_2 s^2 \right]^{11/10} + B_3 s^3 \right\}^{2/15} \tag{25}$$

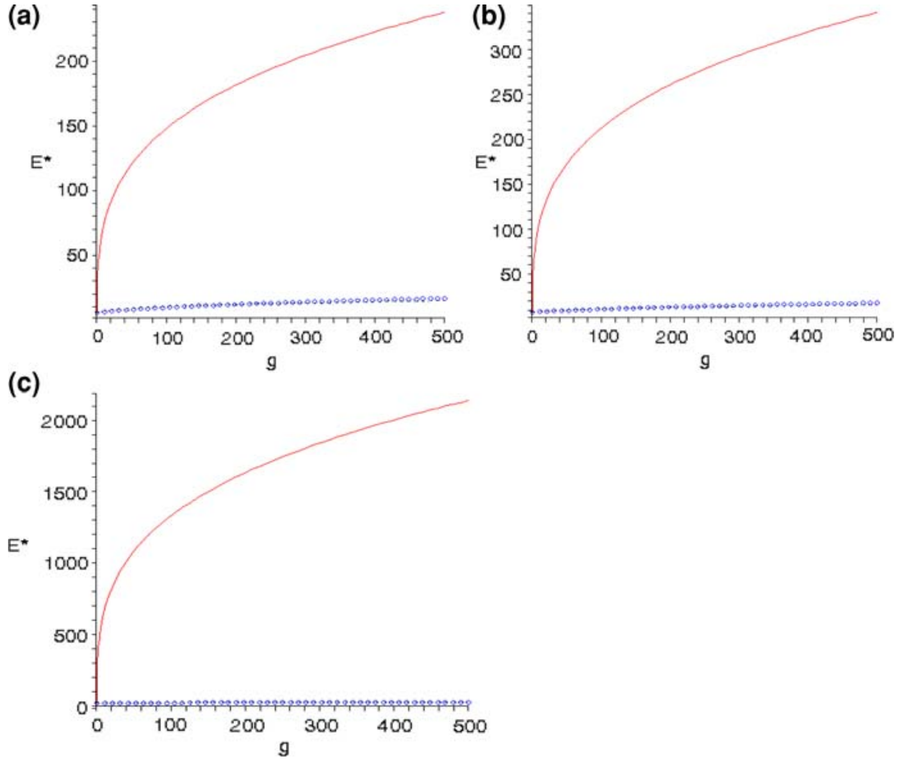

Fig. 3 Percentage errors of the self-similar approximants as functions of the coupling parameter g, in a pancake-shape trap, with $\lambda = 10$. E_1^* (*solid line*), E_2^* (*point line*), and E_3^* (*patch line*) are related with different energy levels: **a** $n = m = k = 0$; **b** $n = k = 0$, $m = 2$; **c** $n = k = 0$, $m = 10$

where

$$B_1 = \frac{(0.25)^{125/22}}{a_0^{125/22}} \left[30\left(\frac{p^2}{2}+\frac{(q\lambda)^2}{4}\right)\right]^{5/66}$$
$$\times \left[\frac{-3p^4+2p^2(q\lambda)^2-2(q\lambda)^4}{\frac{20}{\frac{11}{10}\left(\frac{p^2}{2}+\frac{(q\lambda)^2}{4}\right)}} - \frac{130}{44}\left(\frac{\left(\frac{p^2}{2}+\frac{(q\lambda)^2}{4}\right)}{0.25}\right)\right]^{5/6}$$
$$B_2 = \left(\frac{0.25}{a_0}\right)^{75/11}\left[30\left(\frac{p^2}{2}+\frac{(q\lambda)^2}{4}\right)\right]^{10/11}, \quad B_3 = \left(\frac{0.25}{a_0}\right)^{15/2}.$$

Now, we can analyze graphically the accuracy of the self-similar root approximants $E_k^*(s)$ as function of the coupling parameter g and using the negative effective interaction strength s.

Now we calculate the percentage errors $\varepsilon_k^*(s)$ comparing $E_k^*(s)$ with the controlled approximant in Eq. 14. We have calculated the maximal errors $\varepsilon_k^* \equiv \max_s \varepsilon_k^*(s)$ for the anisotropy parameter λ, defined in Eq. 4, in the range $0.1 \leq \lambda \leq 2000$ for the ground state and for some excited states. For example, for the ground state with $n = m = k = 0$ and for $\lambda = 1$ we have obtained

$$\varepsilon_1^* = 4.1\%, \quad \varepsilon_2^* = 2.1\% \quad \text{and} \quad \varepsilon_3^* = 1.1\%.$$

which demonstrates good convergence. In the case of a cigar shape trap with $\lambda = 0.1$, we have obtained

$$\varepsilon_1^* = 9\%, \quad \varepsilon_2^* = 3.8\% \quad \text{and} \quad \varepsilon_3^* = 1.9\%.$$

For a pancake shape trap with $\lambda = 10$, we have attained

$$\varepsilon_1^* = 12.4\%, \quad \varepsilon_2^* = 3.5\% \quad \text{and} \quad \varepsilon_3^* = 1.9\%.$$

The same good convergence occurs for the excited states with different quantum numbers and for several anisotropy parameters. We showed in Figs. 1, 2 and 3 the percentage errors E_1^*, E_2^* and E_3^* for several levels and different anisotropy parameters. So, the crossover approximants, E_k^*, as functions of the negative coupling parameter, g, are analyzed with more details and precisions.

5 Conclusions

With the controlled perturbation theory method [22], we have found approximate solutions for the spectrum of the cylindrically trapped Bose gas and with influence of the negative values of the coupling parameter. Analytical expressions for the spectrum of the level energies using the negative coupling parameter were obtained by employing the self-similar root approximant method.

The approximations obtained by employing these two methods provided the best accuracy for all negative couplings, g, for the limits of weak and strong couplings of the corresponding asymptotically exact solutions.

Acknowledgments This work was accomplished in The Optics and Photonics Research Center, University of São Paulo, São Carlos. We are grateful to V. Yukalov and E. P. Yukalova for introducing us to the methods here employed and for the very fruitful collaboration along the past years. We appreciate financial support from CAPES and CNPQ (Brazilian agencies).

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