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One-Dimensional Confined Bose Gas in a Quartic Potential: Calculation of the Energy Levels and the Critical Coupling Parameter

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ABSTRACT

Perturbation theory can be reformulated as dynamic theory applied to crystals and gases. Here we concentrate our attention on the stability conditions that allow controlling the convergence of approximation sequences. These ideas are illustrated by calculating the energy levels and critical coupling parameter of a one-dimensional confined Bose gas.

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Introduction

Quantum confined gases are among the most interesting and excite topics of investigation. While most theory and experiments are concerned with three-dimensional systems, we have still many important and surprising aspects for confinements considered to be one-dimension. Nevertheless, dealing with one-dimension system, one always faces the necessity to introduce perturbation on the system.

The main question for any variant of perturbative methods is how to control the convergence if neither an explicit form of high-order approximations nor the exact solutions are available. To overcome this difficulty, an idea has been developed, in which the perturbation algorithm can be supplemented by a set of functions controlling the convergence of the approximation sequence [1]. Those are called the control functions, and they have been first explored and used for describing anharmonic crystals properties [1-6]. Control functions were defined by a minimal-difference condition and have also been applied to several models [2, 7-15]. The choice of conditions for control functions has been mainly heuristic. There are no studies for confined Bose gas in a one-dimensional parabolic potential containing a quartic power term.

To justify the option condition to define the control functions, it was shown that perturbation theory could be formulated as a renormalization group theory [16-20]. With this view, control functions can be defined from a fixed-point condition, whose particular variants yield either the minimal-difference or minimal-sensitivity conditions? As far as a renormalization group can be considered, as a kind of dynamical system, it was natural to reformulate perturbation theory to the language of dynamical theory [21-23]. This reformulation not only makes the theory more logical but also permits to define stability conditions related to the problem convergence. The so-called controlled perturbation theory. Approaches like this can find a great deal of applications in confined Bose-Einstein Condensate (BEC).

In this study, we have demonstrated the method of controlled perturbation theory to the case of a confined Bose gas in an one-dimensional parabolic potential containing a quartic power term. The paper is organized as follows. In Section 2, we formulate the model on perturbation theory, and in Section 3 we start by explaining the method through the application of a confined Bose gas in a quartic potential. In conclusion Section 3, we summarize the results and encourage experimental studies to study such properties in bosonic gases.

Materials and Methods

Dominated (Controlled) Perturbation Theory

Consider that we are interested in the behavior of a real function f(s) where s is a real variable, namely the coupling parameter. The f(s) function can be defined by a complicated equation which not have an exact solution and therefore, only an approximate numerical solution can be found. Nevertheless, we can find the asymptotic expansion

$$\boldsymbol{f(s) = a_o + a_1 s + a_2 s^2 + \cdots \quad (s \to 0)}, \qquad (1)$$

it is, in the weak-coupling limit. On the other hand, we can also derive the asymptotic expansion in the strong coupling limit, in the form

$$f(s) = b_o s^{\beta_0} + b_1 s^{\beta_1} + b_2 s^{\beta_2} + \cdots \quad (s \to \infty), \qquad (2)$$

where $\boldsymbol{\beta_j}$ are arranged in the decreasing order, $\boldsymbol{\beta_j} > \boldsymbol{\beta_j}+1$.

To achieve the fast convergence of the divergent series control functions are implemented through of a multiplicative algebraic transformation and by using also the self-similar approximation, yielding to the self-similar root approximation

$$f_k^*(s) = a_0(\ldots\{[(1 + A_1 s)^{n_1} + A_2 s^2]^{n_2} + A_3 s^3\}^{n_3} + \cdots + A_k s^k)^{n_k}, \qquad (3)$$

where k is the order of the approximation taken, A_j are the coefficients, and n_j are the potences, which are to be defined by considering the strong-coupling limit of the approximant in Eq. (3) and equating it to the strong-coupling expansion in Eq. (2). This way can be called the left-to-right crossover [1, 3-15].

In general, it could be possible to go to the opposite way, i.e., from the right to the left. That is, we could construct a nested-root approximant starting from the strong-coupling asymptotic form of Eq. (2) and then define the corresponding coefficients and powers by equating to the asymptotic expansion of Eq. (1). However, the right-to-left crossover results in approximants usually are less accurate than the left-to-right crossover formulas. This is connected to the fact that the weak-coupling expansions have, as a rule, zero radius of convergence, while the strong-coupling ones have a finite radius of convergence. The accuracy of the left-to-right crossover approximants is usually better than that of the right-to-left ones because of the larger region of applicability of the strong-coupling expansion in Eq. (2) as compared to the region of validity of the weak-coupling expansion in Eq. (1). In fact, the latter can be valid for s≪1, hence its region of validity is inside the interval (0,1). In contrast, the strong-coupling form, derived for s>>1, has the region of applicability inside the interval (1,∞). Therefore, the self-similar crossover approximant must be fitted to the asymptotic expansion that possesses the larger region of validity.

When considering the strong-coupling limit $s \to \infty$ for the approximant of Eq. (3), we need to know the relation between the powers nj and the numbers j=1,2,… Among all possible relations, we must choose that one which is the most general, imposing no restrictions on the powers β_j. It is possible to show that the condition

$$jn_j < j + 1 \quad (j = 1,2, \ldots, k - 1) \qquad (4)$$

provides a general way of expanding the form of Eq. (3), valid for any k=1,2,… and any arbitrary β_j.

Under the criterion of Eq. (4), and rewriting the approximant in Eq. (3) in the form

$$f_k^*(s) = a_0\left(A_k s^k\right)^{n_k}\left(1 + \frac{A_{k-1}^{n_{k-1}}}{A_k} x^{k-(k-1)n_{k-1}} * \left\{+\frac{A_{k-2}^{n_{k-2}}}{A_{k-1}} x^{k-1-(k-2)n_{k-2}}\left(1 + \cdots + \frac{A_2^{n_2}}{A_3} x^{3-2n_2} * \left[1 + \frac{A_1^{n_1}}{A_2} x^{2-n_1}\left(1 + \frac{x}{A_1}\right)^{n_1}\right]^{n_2}\right)^{n_3} \ldots\right\}^{n_{k-1}}\right)^{n_k}$$

where $x \equiv s^{-1}$, it is easy to expand the latter in powers of x. Comparing the resulting expansion with the strong-coupling limit in Eq. (2) we obtain

$$kn_k = \beta_0$$

$$(k - j)n_{k-j} = \beta_j - \beta_{j-1} + k - j + 1, \qquad (5)$$

with $1 \le j \le k-1$. The values of n_j, defined by Eq. (5), are in compliance with the criterion showed in Eq. (4) because of the inequality $\beta_j - \beta_{j-1} < 0$.

The first-order self-similar approximant in Eq. (3) is

$$f_1^*(s) = a_0(1 + As)^{n_1},$$

where $A^{n_1} = {}^{b_0}/_{a_0}$, and $n_1 = \beta_0$.

The second-order approximant in Eq. (3) takes the form

$$f_2^*(s) = a_0[(1 + As)^{n_1} + A_2 s^2]^{n_2},$$

in which

$$f_2^*(s) = a_0[(1 + As)^{n_1} + A_2 s^2]^{n_2},$$

$$A_1^{n_1 n_2} = \frac{b_0}{a_0}\left(\frac{b_1}{n_2 b_0}\right)^{n_2}, \quad A_2^{n_2} = \frac{b_0}{a_0},$$

$$n_1 = \beta_1 - \beta_2 + 2, \quad 2n_2 = \beta_0.$$

In the third order, we find

$$f_2^*(s) = a_0\{[(1 + B_1 s)^{n_1} + B_2 s^2]^{n_2} + B_3 s^3\}^{n_3},$$

where

$$B_1^{n_1 n_2 n_3} = \frac{b_0}{a_0}\left(\frac{b_1}{n_3 b_0}\right)^{n_3}\left(\frac{b_2}{n_2 b_1} - \frac{n_3 - 1}{2n_2 n_3}\frac{b_1}{b_0}\right)^{n_2 n_3},$$

$$B_2^{n_2 n_3} = \frac{b_0}{a_0}\left(\frac{b_1}{n_3 b_0}\right)^{n_3}, \quad B_3^{n_3} = \frac{b_0}{a_0},$$

$$n_2 = \beta_2 - \beta_1 + 2, \quad 2n_2 = \beta_1 - \beta_0 + 3, 3n_3 = \beta_0.$$

The method of constructing self-similar crossover formulas is also applicable to asymptotic expansions more general than showed in Eq. (1), for instance to series

$$f(s) = a_0 + a_1 s^{\alpha_1} + a_2 s^{\alpha_2} + \cdots \quad (s \to 0), \quad (6)$$

in which α_j are arbitrary positive powers arranged in the increasing order as

$$0 < \alpha_j < \alpha_{j+1} \quad (7)$$

Then, instead of Eq. (3), we obtain the self-similar approximant

$$f_k^*(s) = a_0(\ldots\{[(1 + A_1 s^{\alpha_1})^{n_1} + A_2 s^{\alpha_2}]^{n_2} + A_3 s^{\alpha_3}\} + \cdots + A_k s^{\alpha_k})^{\alpha_k} \quad (8)$$

The criterion showed in Eq. (4) transforms to the inequality

$$\alpha_j n_j < \alpha_{j+1} \quad (9)$$

and, in the place of Eqs. (5), we find

$$\alpha_k n_k = \beta_0,$$

$$\alpha_j n_j = \alpha_{j+1} + \beta_{k-j} - \beta_{k-j-1} \quad (10)$$

with j=1,2,…, k – 1.

The described method makes it possible to construct analytical interpolative formulas for the whole range of the coupling parameter. The method can also be used for interpolating any functions of other variables, provided the corresponding asymptotic expansions are available.

Results

Confined Bose Gas in a Quartic Potential

To illustrate the ideas of the approach we have chosen as example a confined Bose gas model. Suppose we need to find the energy levels of a confined Bose gas represented by one-dimensional anharmonic oscillator with the Hamiltonian

$$\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + gx^4 \quad (11)$$

Where x *E* (-∞,∞) and the coupling, or anharmonicity, parameter g ≥ 0. It is worth nothing that several problems of quantum mechanics can be reduced to oscillator-type models by a special change of variables [24, 25].

We also would like to emphasize that our aim here is not simply the calculation of the energy levels but the demonstration of the self-similar perturbation theory [2].

It is natural to start from the confined Bose gas whose Hamiltonian,

$$\widehat{H_0} == -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}u^2 x^2, \quad (12)$$

Which contains an unknown control parameter u. For convenience we introduce the notation

$$E_k(g,u) \equiv \left(n + \frac{1}{2}\right) F_k(g,u) \quad (13)$$

for the k-order approximation of the spectrum. The quantum index n=0,1,2… in E_k and F_k is not written explicitly for the sake of brevity.

The sequence $\{F_k(g,u)\}_{k=0}^{\infty}$ is to be obtained by Rayleigh-Schrödinger perturbation theory starting from

$$F_0(g,u) = u. \quad (14)$$

In that follows we shall need the notation

$$\alpha = \alpha(u) \equiv 1 - \frac{1}{u^2},$$

$$\beta = \beta(u) \equiv \frac{6\gamma g}{u^3},$$

$$\gamma \equiv \frac{n^2+n+1/2}{n+1/2}. \quad (15)$$

The first four approximations, under a fixed u, are

$$F_1(g,u) = u - \frac{1}{4}u(2\alpha - \beta),$$

$$F_2(g,u) = F_1(g,u) - \frac{1}{8}u(\alpha^2 - 2\alpha\beta + 2a\alpha\beta^2), \quad (16)$$

$$F_3(g,u) = F_2(g,u) - \frac{1}{16}u(\alpha^3 - 4\alpha^2\beta + 10a\alpha\beta^2 - 3b\beta^3),$$

$$F_4(g,u) = F_3(g,u) - \frac{1}{32}u\left(\frac{5}{4}\alpha^4 - 8\alpha^3\beta + 35a\alpha^2\beta^2 - 24ab\beta^3 + c\beta^4\right).$$

in which

$$a = a(\gamma) \equiv \frac{17n^2 + 17n + 21}{(6\gamma)^2},$$

$$b = b(\gamma) \equiv \frac{125n^4 + 250n^3 + 472n^2 + 347n + 111}{(n + 1/2)(6\gamma)^3},$$

$$c = c(\gamma) \equiv \frac{10689n^4 + 21378n^3 + 60616n^2 + 49927n + 30885}{8(6\gamma)^4}.$$

$$\beta\frac{\partial}{\partial u_1}F_1(x,u_1) = 0 \quad (17)$$

we get the equation

$$u_1^3 - u_1 - 6\gamma g = 0 \quad (18)$$

as a result of which

$$\alpha = \beta = \frac{u_1^2 - 1}{u_1^2}.$$

Substituting the solution u_1 (g) from Eq. (18), into Eq. (16), we define

$$f_k(g) \equiv F_k(g, u_1(g)). \quad (19)$$

Then, from Eq. (16) we have

$$f_1(g) = \frac{3}{4}u_1 + \frac{1}{4u_1}, \quad f_2(g) = f_1(g) + \frac{1}{8}(1 - 2a)\alpha^2 u_1. \quad (20)$$

In the region of $g>0$, the energy (Eq. 13) is positive for small |g|, and, as g diminishes, the energy becomes zero at a critical value g_c. The latter can be found from the definition

$$f_1(g_c) = 0 \qquad (21)$$

The form of the Eq. (20) shows that equality in Eq. (21) holds true for $u_c^2 = -\frac{1}{3}$. Then, for the ground-state level with $n = 0$, one finds

$$g_c = -0.12830 \qquad (n = 0) \qquad (22)$$

the solution of Eq. (18) needs to satisfy the boundary condition $u_1\,(g)\to 1$, as $g\to 0$. Such a solution is

$$u_1 g = \left(\tfrac{1}{9}\sqrt{729\gamma^2 g^2 - 3} + 3\gamma g\right)^{1/3} + \tfrac{1}{3}\left(\tfrac{1}{9}\sqrt{729\gamma^2 g^2 - 3} + 3\gamma g\right)^{-1/3} \qquad (23)$$

the control function in Eq. (23) is real for $g \le g_n$, where

$$g_n \equiv \frac{g_c}{\gamma} = \frac{n+1/2}{n^2+n+1/2}\, g_c \qquad (24)$$

and complex roots of Eq. (23) appear only after $g \le g_n$ [26, 27].

Asymptotic expansions in the weak- and strong-coupling limits can be written for arbitrary energy levels. For illustrative purpose, we shall write down expansions for the ground state (n=0) and we shall plot the graphics of expansions in function of coupling parameter.

For the ground state, when n=0 and γ=1, function in Eq. 10 yields for the real parts

$$R_e f_1(g) \approx 1 - \frac{3}{2} - \frac{9}{2}g^2 - 27g^3 - \frac{1701}{8}g^4,$$

$$R_e f_1(g) \approx 1 - \frac{3}{2}g - \frac{21}{4}g^2 - \frac{153}{4}g^3 - \frac{729}{2}g^4 \; (n = 0) \qquad (25)$$

while the imaginary parts are

$$Im f_1(g) = Im f_2(g) = 0, \quad g \to 0. \qquad (26)$$

In the strong-coupling limit, when, $g\to\infty$, for the ground state we obtain the real parts

$$R_e f_1(g) \approx \frac{3}{8}(6g)^{1/3} + \frac{1}{4}(6g)^{-1/3} + \frac{1}{12}(6g)^{-1} - \frac{1}{108}(6g)^{-5/3} - \frac{1}{648}(6g)^{-7/3},$$

$$R_e f_2(g) \approx \frac{35}{96}(6g)^{1/3} + \frac{7}{288}(6g)^{-1/3} + \frac{17}{144}(6g)^{-1} - \frac{43}{1944}(6g)^{-5/3} - \frac{211}{23328}(6g)^{-7/3} \qquad (27)$$

And the imaginary parts

$$Im f_1(g) \approx \frac{3\sqrt{3}}{8}(6g)^{1/3} + \frac{\sqrt{3}}{4}(6g)^{-1/3} - \frac{\sqrt{3}}{108}(6g)^{-5/3} - \frac{\sqrt{3}}{648}(6g)^{-7/3},$$

$$Im f_2(g) \approx \frac{35\sqrt{3}}{96}(6g)^{1/3} + \frac{77\sqrt{3}}{288}(6g)^{-1/3} - \frac{43\sqrt{3}}{1944}(6g)^{-5/3} - \frac{211\sqrt{3}}{23328}(6g)^{-7/3}. \qquad (28)$$

Varying the coupling parameter g, we can analyze graphically the behavior of the asymptotic expansions in the weak- and strong-limits for the ground state and calculate the real parts in Figures 1 and 2.

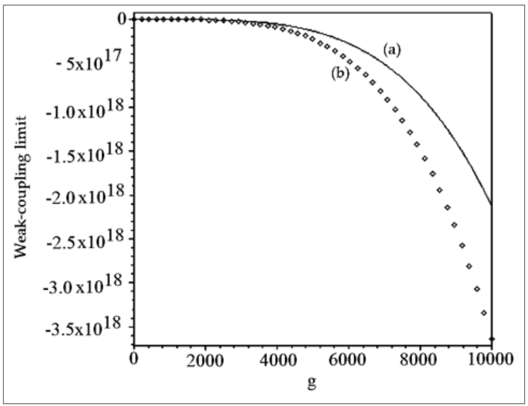

Figure 1: Real parts of the approximations in the weak-coupling limit, a) $R_e f_1$ (g) (solid line) and b) $R_e f_2$ (g) (dashed line) as function of the different values for the coupling parameter (g).

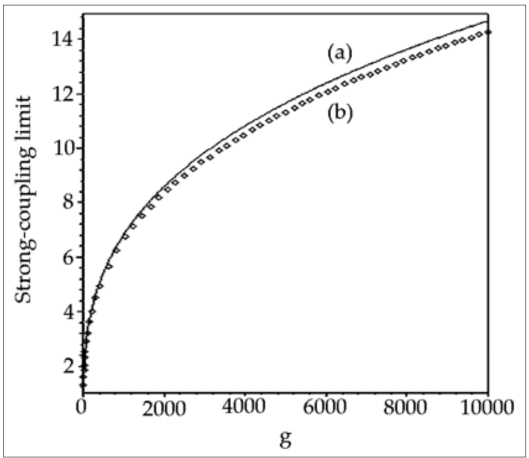

Figure 2: Real parts of the approximations in the strong-coupling limit, a) $R_e f_1$ (g) (solid line) and b) $R_e f_2$ (g) (dashed line) as function of the different values for the coupling parameter (g).

In the strong-coupling limit, when,$g \to \infty$, for the ground state, we obtain graphically the imaginary parts of the approximations for the different values of the coupling parameter g in Figure 3.

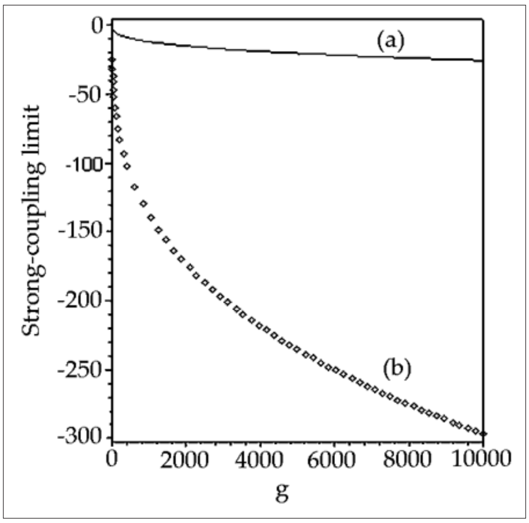

Figure 3: Imaginary parts of the approximations in the strong-coupling limit, a) Imf_1 (g) (solid line) and b) Imf_2 (g) (dashed line) as function of the different values for the coupling parameter (g).

The accuracy of the real parts of the approximations in Eq. (20) is sufficiently good; the maximal error in the first order is -3.3% and in the second order is 2%. In the case of the corresponding imaginary parts, the maximal error for g>g_n is about of 10%.

Conclusions

The knowledge of the ground state energy for non-harmonic potentials is an important challenge, in view of the high possibilities of application that we can have involving Bose condensates. The presence of non-harmonic terms and their influence both on the thermodynamic properties and on the hydrodynamic properties of the system, such as collective modes, and others, creates new possibilities of exploration for trapped quantum gases. In this study, we present the use of the controlled perturbation method to verify the system ground state energy values in one dimension. Despite several ways of calculating the approximate ground state energy when non-harmonic terms are present, the controlled perturbative method allows to obtain a greater degree of precision. Furthermore, the method used here allows its use in situations where the non-harmonic term is not just a small variation of the problem, but situations where the coupling term is arbitrarily large. Thanks to the possibility of introducing control functions, the convergence of the method can be guaranteed. Although we have carried out the proof for the one-dimensional system, the two- and three-dimensional cases can be seen as natural extensions of the problem, despite demanding a little more mathematical concern. An important practical example for us to apply deals with the almost unidimensional confines reached when we have extremely unbalanced cigar traps with extremely high anisotropy. Such traps could, in principle, be obtained experimentally and critical properties of the condensate obtained could be investigated both theoretically and experimentally.

Author Contributions

Conceptualization, V.S.B. and A.G.S.; methodology, A.G.S.; writing—original draft preparation, V.S.B. and A.B.F.S.; writing—review and editing, V.A.N.; visualization, A.C.M.T.; All authors have read and agreed to the published version of the manuscript.

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Not applicable

Data Availability Statement

The data presented in this study are available on request from the corresponding author.

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Conflicts of Interest

The authors declare no conflict of interest.

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