Variational study of dilute Bose condensate in a harmonic trap

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(March 1, 2018)

Abstract

A two-parameter trial condensate wave function is used to find an approximate variational solution to the Gross-Pitaevskii equation for $N_0$ condensed bosons in an isotropic harmonic trap with oscillator length $d_0$ and interacting through a repulsive two-body scattering length $a > 0$. The dimensionless parameter $N_0 \equiv N_0 a/d_0$ characterizes the effect of the interparticle interactions, with $N_0 \ll 1$ for an ideal gas and $N_0 \gg 1$ for a strongly interacting system (the Thomas-Fermi limit). The trial function interpolates smoothly between these two limits, and the three separate contributions (kinetic energy, trap potential energy, and two-body interaction energy) to the variational condensate energy and the condensate chemical potential are determined parametrically for any value of $N_0$, along with illustrative numerical values. The straightforward generalization to an anisotropic harmonic trap is considered briefly.

PACS numbers: 03.75.Fi, 05.30.Jp, 32.80.Pj, 67.40(Db)

I. INTRODUCTION

The remarkable observation of Bose-Einstein condensation of dilute ultracold alkali atoms in a harmonic trap [1-3] has stimulated much theoretical activity, based mostly on the Gross-Pitaevskii (GP) equation [4,5] that is believed to describe accurately the experimental situation well below the onset of Bose-Einstein condensation. In this picture, the two-body
interaction is characterized by the s-wave scattering length $a$ (typically, $a \sim 10$ nm and positive, but $a$ is negative for $^7\text{Li}$ [2]). The actual traps are anisotropic, but, for simplicity, the present work concentrates on an isotropic trap with frequency $\omega_0$ and oscillator length $d_0 = \sqrt{\hbar/m\omega_0}$ (typically, $d_0 \sim$ a few $\mu$m). Although the nonlinear GP equation is readily solved numerically for the selfconsistent wave function $\Psi$ of $N_0$ condensed atoms in an isotropic trap [3,7] with a total of $N$ atoms, it is often useful to have an analytic approximation that provides a semiquantitative description of the condensate density $n_0(r)$ associated with the $N_0 \leq N$ condensed atoms. For example, Baym and Pethick [8] proposed two very different approximations: a Gaussian trial function in the limit of a small condensate ($N_0 \equiv N_0|a|/d_0 \ll 1$) and a Thomas-Fermi (TF) approximation in the limit of a large condensate ($N_0 \equiv N_0|a|/d_0 \gg 1$). The present work studies a simple variational trial function that includes the two limiting cases and yields a useful interpolation for intermediate values of $N_0$.

The basic formalism is reviewed in Sec. II, and the explicit variational trial function is analyzed in Sec. III for positive scattering length $a > 0$. Typical numerical values are presented in Sec. IV, along with the various components of the energy per particle and the chemical potential. The quite different situation for negative scattering length is discussed briefly in Sec. V, and the generalization to an anisotropic harmonic trap is considered in Sec. VI.

II. BASIC FORMALISM

In the special case of a uniform dilute Bose gas at $T = 0$ K subject to periodic boundary conditions, Bogoliubov [9] made the essential observation that the total number of condensed atoms is large ($N_0 \gg 1$). More generally, for a nonuniform condensate, the occupation of the various single-particle states can be characterized by creation and annihilation operators $a_j^\dagger$ and $a_j$ that obey Bose commutation relations $[a_j, a_k^\dagger] = \delta_{jk}$. The condition $N_0 \gg 1$ implies that the operators for the condensate mode can be treated simply as numbers [3,10], because
their commutator \( [a_0, a_0^\dagger] = 1 \) is small compared to their value \( a_0 \approx a_0^\dagger \approx \sqrt{N_0} \). As a result, the condensate is described by a conventional wave function \( \Psi(\mathbf{r}) \) and a “thermodynamic-potential” functional [obtained as a Legendre transformation from the “energy” functional \( E_0(N_0) \)]

\[
K_0(\mu_0) \equiv E_0 - \mu_0 N_0 = \int d^3 r \ |\Psi^* (T + U - \mu_0) \Psi + 2 \pi a^2 \hbar^2 m^{-1} \int d^3 r \ |\Psi|^4 \tag{1}
\]

that gives the dominant contribution for small noncondensate number \( N' \equiv N - N_0 \ll N \).

Here \( E_0(N_0) \) is the condensate energy, \( T = -\hbar^2 \nabla^2 / 2m \) is the kinetic energy and \( U(\mathbf{r}) = \frac{1}{2} m \omega_0^2 r^2 \) is the isotropic harmonic trap potential. The condensate wave function is normalized to the total condensate number

\[
\int d^3 r \ |\Psi|^2 = N_0, \tag{2}
\]

so that the condensate particle density is simply \( n_0(\mathbf{r}) = |\Psi(\mathbf{r})|^2 \); the Euler-Lagrange equation for the functional in Eq. (1) is just the nonlinear Gross-Pitaevskii (GP) eigenvalue equation

\[
(T + U + V) \Psi = \mu_0 \Psi, \tag{3}
\]

where \( V(\mathbf{r}) = 4 \pi a^2 \hbar^2 n_0(\mathbf{r}) / m \) is the mean (pseudo)potential energy per condensed particle. In the present case of a harmonic trap, \( \mu_0 \) must be adjusted to ensure that the wave function obeys the asymptotic boundary condition that \( \Psi \rightarrow 0 \) as \( r \rightarrow \infty \). In addition, \( \mu_0 \) obeys the thermodynamic relation

\[
\mu_0 = \frac{\partial E_0(N_0)}{\partial N_0}, \tag{4}
\]

or, equivalently,

\[
N_0 = - \frac{\partial K_0(\mu_0)}{\partial \mu_0}. \tag{5}
\]

If the exact condensate wave function is known, then the exact condensate energy is given by
\[ E_0 = \langle T \rangle + \langle U \rangle + \frac{1}{2}\langle V \rangle, \]  

(6)

where the angular brackets denote an expectation value evaluated with the condensate wave function (namely, \( \langle \cdots \rangle = \int d^3r \Psi^* \cdots \Psi \)). A combination of Eqs. (4) and (6) gives

\[ \mu_0 N_0 = \langle T \rangle + \langle U \rangle + \langle V \rangle, \]  

(7)

because \( V \) itself is proportional to \( N_0 \) [this last result also follows directly from the GP Eq. (3)].

**III. VARIATIONAL TRIAL FUNCTION**

It is convenient to introduce dimensionless units, with \( d_0 \) and \( \hbar \omega_0 \) as the length and energy scales. In this case, the dimensionless kinetic energy and trap potential energy become \( T = -\frac{1}{2} \nabla^2 \) and \( U = \frac{1}{2} r^2 \). As a simple variational trial function for the isotropic condensate, take

\[ \Psi(r) = c_0 (1 - r^2/R^2)^{(1+\lambda)/2} \theta(R - r) \]  

(8)

that depends on the two dimensionless parameters \( \lambda \) and \( R \). The normalization constant \( c_0 \) follows immediately from Eq. (2)

\[ c_0^2 = \frac{N_0 \Gamma(\frac{7}{2} + \lambda)}{2\pi R^3 \Gamma(\frac{5}{2}) \Gamma(2 + \lambda)}. \]  

(9)

For \( \lambda \to 0 \), the trial function obviously reduces to the TF approximation \( \Psi_{TF}(r) \propto (1 - r^2/R^2)^{1/2} \theta(R - r) \), which follows by neglecting the kinetic energy relative to the trap potential energy and the interparticle potential energy; in this case \( U - \mu_0 + V \) vanishes in the region where \( \Psi \neq 0 \), and \( \mu_0 \approx \frac{1}{2} R^2 \) for an isotropic harmonic trap. The condensate density in this TF limit is parabolic, with \( n_0(r) \propto (1 - r^2/R^2)^{\theta}(R - r) \), showing that \( R \) is the (large) dimensionless TF condensate radius, and it is easy to verify that \[ R^5 \approx 15N_0, \]  

where \( N_0 \equiv N_0 a/d_0 \gg 1 \), and that \( E_0/N_0 \approx \frac{5}{4} \mu_0 \).
The opposite case occurs for $\lambda \to \infty$. In this limit, a detailed analysis (see below) shows that $N_0 \approx \sqrt{32\pi/\lambda} \ll 1$, and that $R \approx \sqrt{\lambda} \gg 1$; in addition, a standard asymptotic identity involving the Gamma function \[11\]

$$\frac{\Gamma(z+a)}{\Gamma(z+b)} \sim z^{a-b} [1 + O(z^{-1})], \quad \text{for } |z| \to \infty,$$

(10)

verifies that the trial function reduces to a normalized isotropic Gaussian with condensate density

$$n_0(r) = |\Psi_G(r)|^2 = N_0\pi^{-3/2} \lim_{\lambda \to \infty} (1 - r^2/\lambda)^{1+\lambda} \approx N_0\pi^{-3/2} \exp(-r^2),$$

as used by Baym and Pethick \[8\] (in this low-density, near-ideal, limit, the condensate density is independent of $R$, and the mean-square condensate radius is $\frac{3}{2}$).

For general $\lambda$ and $R$, the various expectation values are readily evaluated:

$$\langle T \rangle = \frac{3}{4} N_0 A(\lambda) R^{-2}, \quad \text{where } A(\lambda) = (1 + \lambda)(5/2 + \lambda)/\lambda;$$

(11)

$$\langle U \rangle = \frac{3}{4} N_0 B(\lambda) R^2, \quad \text{where } B(\lambda) = (7/2 + \lambda)^{-1}$$

(12)

[\text{note that the mean-square radius } \langle r^2 \rangle \text{ is just } 2\langle U \rangle/N_0 = \frac{3}{2} B(\lambda) R^2, \text{ which depends on both } \lambda \text{ and } R]; \text{ and}

$$\langle V \rangle = 2N_0 N_0 C(\lambda) R^{-3}, \quad \text{where } C(\lambda) = \frac{\Gamma(3 + 2\lambda)}{\Gamma(\frac{7}{2})\Gamma(\frac{9}{2} + 2\lambda)} \left[\frac{\Gamma(\frac{7}{2} + \lambda)}{\Gamma(2 + \lambda)}\right]^2.$$  

(13)

Thus, the variational energy functional becomes

$$\frac{E_0(R,\lambda)}{N_0} = \frac{3}{4} A(\lambda) R^{-2} + \frac{3}{4} B(\lambda) R^2 + N_0 C(\lambda) R^{-3}.$$  

(14)

Since $A$, $B$, and $C$ are all positive, this expression obviously has a minimum for some positive $R$, and the derivative with respect to $R$ immediately gives the condition

$$-AR + B R^5 = 2N_0 C.$$  

(15)

In addition, the derivative with respect to $\lambda$ yields the second condition

$$\frac{3}{4} A'(\lambda) R^{-2} + \frac{3}{4} B'(\lambda) R^2 + N_0 C'(\lambda) R^{-3} = 0,$$  

(16)
where \( C'(\lambda)/C(\lambda) \) is a linear combination of \( \psi \) functions [11]. Eliminating \( N_0/R^3 \) from Eqs. (13) and (16) leads to an explicit equation for \( R \) as a function of \( \lambda \):

\[
R^4 = \frac{A C'/C - \frac{3}{2} A'/A}{B C'/C + \frac{3}{2} B'/B},
\]

and Eq. (15) then gives the corresponding value of \( N_0 \).

**A. Large condensate (\( N_0 \gg 1 \) and \( \lambda \ll 1 \))**

As shown in Sec. IV, these expressions are readily evaluated for any positive \( \lambda \), but it is helpful first to study two limiting cases, where analytic expressions can be obtained. For \( \lambda \ll 1 \) and \( N_0 \gg 1 \), a detailed expansion [11] yields

\[
\frac{C' \lambda}{C} \approx C_0 + C_1 \lambda + \cdots,
\]

where \( C_0 = \frac{3}{7} \) and \( C_1 = -\frac{2}{3} \pi^2 + \frac{53}{9} + \frac{8}{49} \approx -0.04432 \), so that \( \frac{C'}{C} + \frac{3}{2} B'/B \approx (C_1 + \frac{6}{49}) \lambda + \cdots \). It is then easy to obtain the explicit result

\[
R^4 \approx \frac{105}{8 (C_1 + \frac{6}{49}) \lambda^3}, \quad \text{or} \quad R \approx 3.600 \lambda^{-3/4},
\]

along with \( n_0(r) = |\Psi_{TF}(r)|^2 \approx \lambda^5 (N_0/\pi R^3) (1 - r^2/R^2) \) and the specific results \( \mu_0 \approx \frac{1}{2} R^2 \), \( E_0/N_0 \approx \frac{5}{14} R^2 \), and \( N_0 \approx \frac{1}{15} R^5 \) given in the paragraph below Eq. (13).

**B. Small condensate (\( N_0 \ll 1 \) and \( \lambda \gg 1 \))**

In the opposite limit \( \lambda \gg 1 \) and \( N_0 \ll 1 \), it is simpler to return to Eq. (13), whose solution is of the form \( R(N_0) \approx R_0 + (C/2A) N_0 + \cdots \) with \( R_0^4 = B/A \). To first order in \( N_0 \ll 1 \), the condensate energy is simply

\[
\frac{E_0(\lambda)}{N_0} \equiv \frac{E_0[R_0(\lambda), \lambda]}{N_0} \approx \frac{3}{2} \sqrt{A(\lambda)B(\lambda)} + \frac{C(\lambda) N_0}{R_0(\lambda)^2}.
\]

A direct expansion shows that \( A(\lambda)B(\lambda) \approx 1 + \frac{5}{4} \lambda^{-2} + \cdots \), \( R_0(\lambda) \approx \sqrt{\lambda} (1 + \frac{7}{4} \lambda^{-1} + \cdots) \), and \( C(\lambda) \approx \lambda^{3/2} (2\pi)^{-1/2} (1 + \frac{99}{16} \lambda^{-1} + \cdots) \); thus,
\[ \frac{E_0(\lambda)}{N_0} \approx \frac{3}{2} + \frac{15}{8} \lambda^2 + \cdots + \frac{N_0}{\sqrt{2\pi}} \left(1 - \frac{15}{16} \lambda + \cdots\right) \]  

(21)

This expression clearly has a minimum as a function of \( \lambda \), occurring at

\[ N_0 \approx \frac{\sqrt{32\pi}}{\lambda}; \]  

(22)

the corresponding condensate energy

\[ E_0(N_0) \approx N_0 \left(\frac{3}{2} + \frac{N_0}{\sqrt{2\pi}} + \cdots\right) \]  

(23)

precisely reproduces that found directly for the isotropic normalized gaussian trial function

\[ \Psi_G(r) = \sqrt{N_0} \pi^{-3/4} \exp(-\frac{1}{2}r^2) \]  

[8,12].

### IV. NUMERICAL RESULTS

For any positive value of the variational parameter \( \lambda \), it is straightforward to evaluate the other dimensionless variational parameter \( R \) from Eq. (17), the interaction parameter \( N_0 = N_0 a/d_0 \) that specifies the condensate number from Eq. (15), and the various contributions to the condensate energy per particle and the condensate chemical potential. Typical results are shown in Table 1, illustrating the continuous interpolation between the TF limit (large condensate with \( N_0 \gg 1 \) and \( \lambda \ll 1 \)) and the Gaussian limit (small condensate with \( N_0 \ll 1 \) and \( \lambda \gg 1 \)). In the TF limit, the small-\( \lambda \) approximation in Eq. (19) yields \( R \approx 113.8 \) for \( \lambda = 0.01 \), with the following TF values \( \mathcal{N}_0 \approx \frac{1}{13} R^5 \approx 1.275 \times 10^9 \) and \( \mu_0 \approx \frac{1}{2} R^2 \approx 6480 \); these values are close to the respective variational ones 114.4, 1.297\times10^9, and 6526 given in Table 1. Similarly, the Gaussian (large-\( \lambda \)) limit takes \( R \approx \sqrt{\lambda} \); for \( \lambda = 100 \), this relation gives \( R = 10 \), and the approximate expressions in Eqs. (22) and (23) yield \( N_0 \approx 0.100 \) and \( E_0/N_0 \approx 1.540 \), which should be compared to the respective variational values 0.105 and 1.541 from Table 1 (which also yields the mean-square radius \( \approx 1.56 \), close to that for the ideal gas). Note that the physical parameter \( N_0 \equiv N_0 a/d_0 \) is a single-valued function of \( \lambda \) that decreases monotonically with increasing \( \lambda \).
As an example of the utility of this variational approach, consider the situation for \( \lambda = 1 \), where the ratio \( \langle T \rangle / \langle E_0 \rangle \approx 0.022 \) is already small (so that \( \mu_0 \approx \langle U + V \rangle / N_0 \)), yet the variational condensate density \( |\Psi_{\lambda=1}|^2 \propto (1 - r^2/R^2)^2 \) differs greatly from the parabolic TF condensate density \( |\Psi_{TF}|^2 \propto 1 - r^2/R^2 \). Thus the elementary criterion \( \langle T \rangle / \langle E_0 \rangle \ll 1 \) alone is insufficient to ensure that the condensate density approaches the TF form.

It is important to recall that the variational method provides only an upper bound for the total condensate energy, so that the separate contributions are not necessarily accurate. In particular, Dalfovo, Pitaevskii, and Stringari [13] have used a boundary-layer formalism to show that the kinetic energy per particle in the TF limit is \( \propto R^{-2} \ln R \), which differs significantly from that found variationally.

V. BEHAVIOR FOR NEGATIVE SCATTERING LENGTH

The stability of a Bose condensate with negative scattering length has become of interest in connection with the experimental study of \( ^7 \text{Li} \) [2]. It is well known that a uniform Bose condensate is unstable for arbitrarily small negative interactions (the speed of sound becomes imaginary [3,10]); this behavior is somewhat reminiscent of Jeans’s long-wavelength (gravitational) instability for an infinite uniform stationary medium [14], where the dispersion relation is simply that for a bulk plasma oscillation with the sign of the interaction reversed. The external confining trap completely alters the situation, however, for it eliminates wavelengths longer than the characteristic dimension of the trap (like electromagnetic standing waves in a cavity). Indeed, the Bogoliubov dispersion relation for a uniform medium with negative scattering length \(-|a|\) becomes \[ E_k^2 = (\hbar^2 k^2/2m)^2 (k^2 - 16\pi |a| n_0), \]
which is stable only for wavenumbers greater than \( k_c = \sqrt{16\pi |a| n_0} \). For an order-of-magnitude estimate, take uniform density and \( k_{\text{min}} \approx \pi/2d_0 \) (appropriate for a spherical square well of radius \( d_0 \)); the condition \( k_{\text{min}} > k_c \) yields the approximate stability criterion \( |N_0| < N_{0c} \equiv N_0 |a| / d_0 = \pi^2 / 48 \approx 0.206 \). For comparison, a numerical study of the GP equation for negative scattering length in an isotropic harmonic trap [7] yields the exact
critical value $N_{0c} = 0.573$.

In the present context, it is interesting to examine how the variational calculation treats a negative scattering length. Since the trap can remain stable at $T = 0$ K only for relatively small condensates, it is appropriate to consider the behavior for small negative values of $N_0$. Equation (21) remains valid, but the altered sign of $N_0$ means that $E_0(\lambda)$ achieves its minimum only for $\lambda \to \infty$, corresponding to a Gaussian trial function. This particular situation has already been examined in [12,15], where the local minimum in the variational energy has been shown to disappear at the critical value $|N_{0c}| = (8/25\sqrt{5})^{1/2} \approx 0.671$, somewhat larger than the exact value found numerically in [7].

VI. ANISOTROPIC HARMONIC TRAP

The variational approach has the appealing feature that it is readily generalized to an anisotropic harmonic trap potential, with

$$U(r) = \frac{1}{2}m \sum_j \omega_j^2 r_j^2,$$

where $j = 1, 2$, and $3$ runs over the three coordinate axes. Correspondingly, the three (in general, distinct) oscillator lengths are given by $d_j^2 = \hbar/m\omega_j$. As a natural trial function, take

$$\Psi(r) = c_0 \left(1 - \sum_j \frac{r_j^2}{d_j^2 R_j^2}\right)^{(1+\lambda)/2} \theta\left(1 - \sum_j \frac{r_j^2}{d_j^2 R_j^2}\right),$$

where $\{R_j\}$ is a set of three dimensionless variational parameters. The normalization constant is easily evaluated with Eq. (2) by going to “scaled” variables $x_j = (r_j/d_j R_j)$, yielding the generalization of Eq. (4)

$$c_0^2 = \frac{N_0 \Gamma\left(\frac{7}{2} + \lambda\right)}{2\pi R_1 R_2 R_3 \Gamma\left(\frac{3}{2}\right) \Gamma(2 + \lambda)}. \tag{26}$$

The three relevant expectation values are also readily found for this more general trial function.
\[ \langle T \rangle = \frac{1}{4} N_0 A(\lambda) \sum_j \frac{\hbar \omega_j}{R_j^2}, \]  
\[ \langle U \rangle = \frac{1}{4} N_0 B(\lambda) \sum_j \hbar \omega_j R_j^2, \]  
and
\[ \langle V \rangle = 2N_0 \hbar \omega \frac{N_0 C(\lambda)}{R_1 R_2 R_3}, \]  
where \( \bar{\omega} \equiv \omega_1 \omega_2 \omega_3, N_0 \equiv N_0 a/(d_1 d_2 d_3)^{1/3}, \) and the functions \( A, B, \) and \( C \) are the same as for an isotropic trap, given in Eqs. (11)–(13). Thus, the general variational energy functional
\[ \frac{E_0(\mathbf{R}, \lambda)}{N_0} = \frac{1}{4} N_0 A(\lambda) \sum_j \frac{\hbar \omega_j}{R_j^2} + \frac{1}{4} N_0 B(\lambda) \sum_j \hbar \omega_j R_j^2 + N_0 \hbar \omega \frac{N_0 C(\lambda)}{R_1 R_2 R_3} \]  
depends on the four variational parameters \( R_1, R_2, R_3, \) and \( \lambda. \)

It is not difficult to minimize this functional with respect to each of the first three parameters. The three conditions \( \partial E_0/\partial R_j = 0 \) yield the equations
\[ -A/R_j^2 + BR_j^2 = 2D\bar{\omega}/\omega_j, \]  
where \( D \equiv N_0 C(\lambda)/R_1 R_2 R_3 \) is the same in each equation. This set of conditions can be solved formally to express \( R_j^2 \) as
\[ R_j^2 = \frac{\bar{\omega}D}{\omega_j B} + \sqrt{\frac{A}{B} + \left( \frac{\bar{\omega}D}{\omega_j B} \right)^2}, \]  
where the sign of the root is chosen to give the correct limit for \( a \to 0 \) (the ideal gas). Since \( D^2 = (N_0 C)^2/R_1 R_2 R_3 \), these expressions immediately provide one relation between \( D \) and \( \lambda. \) In addition, the minimum condition \( \partial E_0/\partial \lambda = 0 \) can be combined with Eqs. (31) and (32) to provide a second relation between \( D \) and \( \lambda, \) thus determining both quantities, as well as the three dimensionless parameters \( R_j \) and \( N_0. \) Edwards et al. [16] and Dalfovo and Stringari [17] have used distinct numerical procedures to evaluate the ground-state condensate wave function for anisotropic but axisymmetric traps, using the physical parameters appropriate to [1]; it would be interesting to compare the present variational approach with their explicit results, but such a numerical study remains to be performed.
ACKNOWLEDGMENTS

I am grateful to D. Rokhsar for valuable comments and suggestions. This work was supported in part by the National Science Foundation, under Grant No. DMR 94-21888.
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TABLES

TABLE I. Typical variational physical parameters that characterize a spherical condensate in an isotropic harmonic trap

| $\lambda$ | $R$     | $N_0$     | $\langle T \rangle / N_0$ | $\langle U \rangle / N_0 = \frac{1}{2} \langle r^2 \rangle$ | $\frac{1}{2} \langle V \rangle / N_0$ | $E_0 / N_0$ | $\mu_0$     |
|----------|---------|-----------|---------------------------|-------------------------------------------------|---------------------------------|-------------|-------------|
| 0.01     | 114.407 | 1.2974×10^9 | 0.0145                   | 2796.77                                        | 1864.51                         | 4661.29     | 6525.80     |
| 0.1      | 21.2428 | 2.685×10^5  | 0.0475                   | 94.0115                                        | 62.6426                         | 156.702     | 219.344     |
| 1        | 5.3967  | 153.92     | 0.1803                   | 4.8541                                         | 3.1159                          | 8.1503      | 11.2662     |
| 10       | 4.3724  | 1.5756     | 0.5394                   | 1.0621                                         | 0.3484                          | 1.9499      | 2.2984      |
| 100      | 10.3758 | 0.1054     | 0.7212                   | 0.7801                                         | 0.0393                          | 1.5406      | 1.5799      |