

Sum-rule approaches to the elementary excitation spectrum of interacting gases of finite bosons in harmonic potentials

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Abstract. Based on the corrected sum rules and generalized virial identities, we derive an expression for all modes of excitation spectrum of interacting Bose gases at finite atom numbers in axially anisotropic potentials, in terms of the N -body ground state average. Using the variational Gaussian calculation for the ground-state wave function, its explicit analytic formulas are obtained. These results show clearly the dependence of excitation spectrum on the interaction strength parameter $p = \sqrt{2/\pi}(a_{sc}/a_{ho})(N - 1)$ and trap geometry parameter λ for the system with $N = 1$ through $N \rightarrow \infty$. For $\lambda = 0$ and 1 the dependences have simple and intuitive physical interpretations. We compare the low-lying excitation spectra with the existing numerical results and make quantitative predications for future experiments and numerical simulation for higher-lying excitation modes.

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1 Introduction

Theoretical studies on quantum system show that a combination of microscopic and macroscopic approaches is needed essentially. Experimental studies on Bose-Einstein condensate (BEC) [1] are concentrated in the quantum system of interacting Bose gases in external potentials. For the interatomic interaction in a simple delta-function form, the many-body quantum problem is interesting but complicated. Without external potentials, the problem was solved exactly by use of Bethe ansatz [2] in the one-dimensional (1D) cases; while in the 2D cases the problem became complex and was solved exactly [3]. In the cases with external potentials, however, since the Hamiltonian has off-diagonal terms and the momentum is not a conserved quantity, it is impossible up to now to treat this problem exactly. In some special cases, such as in the Thomas-Fermi limit of atom number $N \rightarrow \infty$, the non-linear Schrödinger equation was solved exactly by [4] with spherical trap and by [5,6] with axial trap. The shift of the elementary excitation spectrum (EES) has been studied in [7,8] due to the chemical potential change, kinetic energy effect, and finite oscillation amplitude. In the opposite case for the weak interacting limit, the EES has also been calculated [9]. In the case of finite N , the analytic expressions for the EES only included three eigenmodes [10]. In that case for some lower excited states, the most successful microscopic approaches have been found to be the

selfconsistent numerical calculations [11–16]. These methods give very detailed, but purely numerical, description of the EES. Alternatively, to gain a better physical insight, macroscopic approaches have been studied [4,17,18]. The approaches of energy-weighted sum rules and moment-weighted virial identities provide a rigorous and powerful tool to connect the microscopic interactions and macroscopic properties of the EES for some collective excitation modes. Simple and closed expression for low-lying modes of the EES are given, that allow for their evaluation from the ground-state wave function.

The usual sum rule is the most popular sum rule and has been the object of many theoretical investigations in the past in atomic physics, quantum mechanics, quantum liquid, superfluidity and nuclear physics [19]. If the spectral density of the response function corresponding to the excitation operator is a delta function, then the sum rule determines exactly the excited energy level. In practice the spectral density is localized about one energy level it only gives the average energy of the collective excitations. Usually the sum-rule approaches can be able to give true results for the EES in a few of lowest excited modes. While in the higher excited modes it gives an uncertain prediction since the spectral density becomes smooth. If the spectral densities have sharp peaks but one doesn't know where the peak positions are at, then the approaches are useless. For example, in a 1D single-body quantum system with harmonic potential, the usual sum rule becomes invalid for most excited states with various choices of the forms of excitation operator. The corrected sum rule [18] solves this

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problem very well with a generalized form of excitation operator. In evaluating the sum rule, we need to calculate the moment-weighted expectation values associated with the system Hamiltonian. Especially the two-fold calculation associated with the interaction energy is very difficult. The usual virial identity only gives the expectation-value relation between kinetic energy, potential energy and interaction energy; while the generalized virial identity [18] may give the moment-weighted expectation-value relation among them.

In this paper, we study the corrected sum rule and generalized virial identity in more detail, and apply them to the entire EES of interacting gases of finite bosons in harmonic potentials. The choice of excitation operator determines the mode being excited. The evaluations of the sum rules associated with the terms of kinetic energy and interaction energy dependent strong on the interaction strength for almost all excitation modes. We extend the usual sum rule in some low-lying modes to all modes by correcting the cubic energy-weighted sum rule. The corresponding terms in the sum rules include two parameters: the relative shift associated with the kinetic energy and enhancement factor associated with the interaction energy. In the special case of $N = 1$, the EES has the exact result after the shift correction. In the opposite case of $N \rightarrow \infty$, the approximate analytic result is as a boundary condition. The controlling of asymptotic behavior determines uniquely the relative shift and enhancement factor, and the corrected sum rule estimate has the reasonable results for all modes in the whole regime of N . The contribution of the interaction energy to the cubic energy-weighted sum rules in two-fold integral expression is equal to the contribution of the kinetic and external field energies in one-fold integral expressions. The goal of this work is to obtain the analytic expression for the entire modes of the EES of interacting gases at finite trapped atom numbers, and get the explicit analytic formulas using the Gaussian variation calculation for the N -body ground-state wave function of the condensate.

This paper is organized as following. In Section 2 we present the theoretical framework at finite trapped atom numbers, deduce the general expression for the sum rules and emphasize the necessity both for the correction on the usual sum rules and for the generalization of the usual virial identity for the entire EES. In Section 3 we derive the analytic expressions for the EES with three symmetric harmonic-oscillator potentials, and give the explicit analytic expressions for the EES by the variational method for the N -body ground-state wave function. Conclusion is in Section 4.

2 Theory descriptions

For a N -body interacting Bose condensed gas in a 3D external harmonic potential $U(\mathbf{r}) = M\omega_{\perp}^2(s^2 + \lambda^2 z^2)/2$, we assume a two-body interatomic interaction of the form $V(\mathbf{r}) = g\delta(\mathbf{r})$ with the coupling constant $g = 4\pi\hbar^2 a_{sc}/M$ fixed by the s -wave scattering length a_{sc} . Where M is the atom mass, ω_{\perp} is the harmonic oscillator frequency in the

xy -plane, and λ is the frequency ratio of the z -axis to the xy -plane in case of the axially symmetric trap with $s^2 = x^2 + y^2$. The system Hamiltonian can be described as

$$\hat{H} = \sum_{i=1}^N \left(\frac{-\hbar^2}{2M} \nabla_i^2 + U(\mathbf{r}_i) \right) + \sum_{i<j}^N g\delta(\mathbf{r}_i - \mathbf{r}_j). \quad (1)$$

Let $|N\rangle_0$ be its ground state at energy E_0 and $|N\rangle_n$ be its n th excited state at energy E_n , the elementary excitation energies are $\hbar\omega_n = E_n - E_0$. Where the quantum numbers n represent the excitation modes of the EES.

For finding analytic expression for ω_n as a function of atom number N , interaction strength g and the trap geometry parameter λ for any excitation modes, one of the best approaches is the sum rule [18,19]. In this section we use n for general quantum numbers to identify the set of excitation modes in the entire excited states. The energy-weighted sum rule, S_1 , and cubic energy-weighted sum rule, S_3 , are defined as

$$S_k = \sum_{n=0}^{\infty} \left| \langle N | \hat{F} | N \rangle_n \right|^2 (\hbar\omega_n)^k, \quad (k = 1, 3) \quad (2)$$

with a collective excitation operator $\hat{F} = \sum_{i=1}^N f(\mathbf{r}_i)$ for the N -body system. The one-body operator $f = f(\mathbf{r}_i)$ can be either a multipole or a plane wave operator depending on the physical problem under consideration. For exciting a general set of modes, the choice of the form f depends on the potential symmetry and corresponding quantum numbers. By defining operator \hat{G} through commutator $\hat{G} = -(2M/\hbar^2)[\hat{H}, \hat{F}]$, one has $\hat{G} = \sum_{i=1}^N \{(\nabla^2 f) + 2(\nabla f) \cdot \nabla\}$ due to the contribution only from the kinetic energy term of the Hamiltonian. It is shown that S_1 is model independent

$$S_1 = \frac{-\hbar^2}{2M} \langle [\hat{F}^+, \hat{G}] \rangle_0 = \frac{\hbar^2}{2M} \langle |\nabla f|^2 \rangle_0, \quad (3)$$

and that S_3 is in terms of a double commutator involving the system Hamiltonian

$$S_3 = \frac{\hbar^4}{2M^2} \left\langle \left[\frac{1}{2} \hat{G}^+, \left[\frac{1}{2} \hat{G}, \hat{H} \right] \right] \right\rangle_0. \quad (4)$$

Where the average $\langle \dots \rangle_0 \equiv {}_0 \langle N | \dots | N \rangle_0$ is taken on the N -body ground state $|N\rangle_0$ with a N -fold integral in real space and runs over all atoms for summation in the discrete form. Since the density Hamiltonian (1) contains three energy terms, potential energy U , interaction energy V , and kinetic energy T , S_3 in equation (4) consists with the corresponding three parts, $S_3 = S_U + S_V + S_T$. U and V 's contributions to S_3 take the same form

$$S_U = \frac{\hbar^4}{2M^2} \langle (\nabla f^*) \cdot (\nabla \{ (\nabla f) \cdot (\nabla U) \}) \rangle_0, \quad (5)$$

and $S_V = (\hbar^4/2M^2) \langle (\nabla f^*) \cdot (\nabla \{ (\nabla f) \cdot (\nabla V) \}) \rangle_0$ because U and V are only as a function of the displacement in real space \mathbf{r} . Where the average $\langle \dots \rangle_0 = {}_0 \langle N | \dots | N \rangle_0$ runs

over all atoms for $i < j = 1, 2, \dots, N$ with $V = g\delta(\mathbf{r}_i - \mathbf{r}_j)$. From $V = 0$ at the boundary of the system, Appendix A proves

$$S_V = \frac{\hbar^4}{2M^2} \langle g\delta(\mathbf{r}_i - \mathbf{r}_j) \{ (\nabla^2 f) (\nabla^2 f^*) + (\nabla f) \cdot (\nabla \nabla^2 f^*) \} \rangle'_0. \quad (6)$$

This is a two-fold summation for $i < j = 1, 2, \dots, N$ and a N -fold integral in 3D real space. For some special modes in which $\nabla^2 f = 0$ we have $S_V = 0$. There is no contributions to the cubic sum rule of the interaction energy for these modes. Carrying out the straightforward algebra, the kinetic energy's contribution to S_3 is written as

$$S_T = \frac{\hbar^6}{4M^3} \left\langle \left\{ -\frac{1}{2} (\nabla \nabla^2 f^*) \cdot (\nabla \nabla^2 f) + \frac{1}{2} (\nabla f^*) \cdot (\nabla \nabla^4 f) + [(\nabla f^*) \cdot \nabla, (\nabla \nabla^2 f) \cdot \nabla] + \left[\frac{1}{2} (\nabla^2 f^*) + (\nabla f^*) \cdot \nabla, [\nabla^2, (\nabla f) \cdot \nabla] \right] \right\} \right\rangle'_0. \quad (7)$$

In the usual sum-rule approaches, the EES can be calculated by the estimate [19] $(\hbar\omega_{n_f})^2 \simeq S_3/S_1 = (S_U + S_V + S_T)/S_1$ when the spectral density or summation kernel in S_3 has a sharp peak at the position of $\omega = \omega_{n_f}$ for choosing f to excite (n_f) th excitation state. The sum-rule approach has at least two points in advances: it only uses the knowledge of the ground states in the system; it provides useful information of the dynamic behavior in the analytic form. Of course, it only gives the estimates by the use of the method similar to the higher Green function approximation.

There is a few system that is exactly solvable in the many-body quantum mechanism. An energy-dependent operator \hat{F} is in such form that $\hat{F}|N\rangle_n$ is an eigenstate of the system. From $[\hat{F}, \hat{H}] = 0$ the EES formula can be obtained by various traditional methods. The sum-rule approaches are invalid since $\hat{G} \propto [\hat{F}, \hat{H}] = 0$, $S_1 \propto \langle [\hat{F}^+, \hat{G}] \rangle_0 = 0$ and $S_3 \propto \langle [\hat{G}^+, [\hat{G}, \hat{H}]] \rangle_0 = 0$ for any excitation states. But sometimes the sum-rule approaches are exact if the excitation operator \hat{F} is chosen in such a way that $\hat{F}^+|N\rangle_n = F_{0n}\delta_{n,n_f}|N\rangle_n$ in the definition of S_k in equation (2) for the (n_f) th excitation state with F_{0n} the matrix elements of \hat{F} , and if expectation values of commutators such as equations (3) and (4) are taken in the exact ground state. For practical system with the sum rule, one usually makes approximations both for the excitation operator \hat{F} which excites some interacting states, and for the ground states which doesn't know exactly in general. In other words, when one doesn't find the single excitation at $n = n_f$, we choose \hat{F} in such a way that $\hat{F}^+|N\rangle_n = F_{0n}|N\rangle_n$ for some excitation states around $n = n_f$ and $F_{0n} \ll F_{0n_f}$ for $n \neq n_f$ where the quantum states $\{n\}$ are interacting with the quantum state n_f and a lot of other noninteracting states don't be excited. In the analytic expression for the EES we assume that the

wave function is the exact ground state that depends on all the particle coordinates.

The estimate of S_3/S_1 and its correction can also be understood by the continuous form of equation (2), $S_k = \int_0^\infty |F_{0n_f}(\omega)|^2 (\hbar\omega)^k \rho \, d\omega = \int_0^\infty \chi''(\omega) (\hbar\omega)^k \, d\omega$ ($k = 1, 3$). Here ρ is the density of states dependent on dimension and choice of coordinates of the system. $F_{0n_f}(\omega)$ is the matrix elements of \hat{F} in the continuous form of excitation energies and $\chi''(\omega)$ is the imaginary part of an appropriate response function. Sum rules are exact if the matrix elements are taken in the exact ground state and are a delta function at $\omega = \omega_{n_f}$. In practice the spectral densities are not delta functions since we can't find a such excitation operator. The sum-rule approaches are not exact even if the commutators in equations (3) and (4) are taken in the exact ground state. If the spectral density functions in S_k have sharp peaks at the frequencies ω_{n_f} for the (n_f) th excitation state, then $S_k \propto (\hbar\omega_{n_f})^k$ and $S_3/S_1 = (\hbar\omega_{n_f})^2$. In the usual sum-rule approaches, the choice of f for the special (n_f) th excitation state always leads the spectral density to be sharply peaked at $\omega = \omega_{n_f}$. Therefore the EES can be calculated by the estimate [19] $(\hbar\omega_n)^2 \simeq S_3/S_1$. In general, however, the spectral density involves some non-quantum background that deduces $S_3/S_1 \neq (\hbar\omega_{n_f})^2$ for the entire modes $\{n_f\}$ with various choices of f form. The correction on the usual sum rule is necessary in most cases. Although we don't know exactly the spectral density functions in practical system since $|N\rangle_n$ still is unknown, we may assume that the spectral density is sharply peaked around ω_{n_f} theoretically after generalizing the form of f to all modes, the cost is to correct S_3 into S_3^c in very clear physical meanings. In that way we will find that the ratio S_3^c/S_1 provides an upper bound to the frequency ω_n of mode n (here and hereafter we note $n = n_f$). In other words, for estimating the EES for the entire excitation modes within the framework of the sum-rule approaches, we are choosing a suitable form of f for showing the nature of the excitation mode, looking at the ratio in two limits $N \rightarrow 1$ and $N \rightarrow \infty$, and observing what corrections must be made to S_3 in order to recover the known limiting mode frequencies, on the basis of the control theory for the asymptotic behavior of the EES. This is the original motivation with the usual physical methodology.

In fact we need to correct S_T and S_V and no need for correction for S_U since the kinetic energy dominates the dynamic process at the weak interacting limit, the interaction energy dominates at the strong interacting limit, while S_U is proportional to S_1 simply and the potential energy takes effect in the whole regime of N . How to correct S_T and S_V ? For some special modes, such as the surface modes in the spherically symmetrical potential, the Laplacian of the excitation operator vanishes. From equations (6) and (7) one has $S_V = 0$ and $S_T = (\hbar^6/4M) \langle [(\nabla f^*) \cdot \nabla, [\nabla^2, (\nabla f) \cdot \nabla]] \rangle_0 \neq 0$ for $\nabla^2 f = 0$. This implies in general that there had better is a shift δS_T for correcting S_T and a multiplicative factor β for correcting S_V , i.e., $S_T^c = S_T - \delta S_T$ and $S_V^c = \beta S_V$. In that corrections, the general expression for the EES at

any trapped atom numbers is

$$(\hbar\omega_n)^2 = (S_U + S_T^c + S_V^c)/S_1. \quad (8)$$

$\omega_n(N)$ as a function of N has two limiting cases: $\omega_n(1)$ and $\omega_n(\infty)$. At $N = 1$, $S_V = 0$ and $\omega_n(1)$ is well-known exact solutions while at $N \rightarrow \infty$, $S_T = 0$ and $\omega_n(\infty)$ has known approximate solutions. As two boundary conditions, $\omega_n(1)$ and $\omega_n(\infty)$ in equation (8) determine independently the parameters δS_T and β after choosing a suitable form of f and carrying out the one-fold and two-fold integrals in equations (5–7). Fortunately, if the shift correction is to drop the constant spectral density in S_T , then $\omega_n(N)$ from equation (8) is exact at $N = 1$ limit. This is because the quantum fluctuation effects to the ground state confine to retain the gradient operator and to cancel the constant operator in the spectral density of S_T . In $N \rightarrow \infty$, the Gross-Pitaevskii equation has explicit analytic eigenvalue solution $\omega_n(\infty)$ for the low-lying excitations; Bogoliubov equations have full numerical solution $\omega_n(\infty)$ for the high-lying excitations. Although we don't know exactly the limiting results of $\omega_n(\infty)$, we can determine β by an approximate results of $\omega_n(\infty)$, on the basis of the control theory for the asymptotic behavior if one assumes that $\omega_n(N)$ has the monotonically asymptotic behavior near the boundary of $N \rightarrow \infty$. The corrected sum rules are valid over the whole range from small to large atom numbers, and the results agree exactly with the harmonic oscillator in single-body limit and agree well with the Thomas-Fermi results in the strong interaction limit for the entire excitation modes of a Bose-Einstein condensate. Therefore, the analytic results of equation (8) in the middle ranges will be useful.

The expectation-value calculation of S_V in equation (6) is more complex, since it integrates in two folds in the continuous forms of V and f . To avoid the difficulty except for $\nabla^2 f = 0$, we will use the generalized virial identities. The detail is given in the Appendix B. In that way V 's contribution to S_3 will be substituted by U 's and T 's contributions and this is a reduced dimension method from two-fold to one-fold integrals in mathematics.

3 Theory calculations

For carrying out the corrected sum rules, generalized virial identities and general calculations of $\tilde{\omega}_n(N) \equiv \omega_n(N)/\omega_\perp$ for different traps, we consider three symmetries of harmonic-oscillators: 3D spherical symmetry, 2D circular symmetry and 3D cylindrical symmetry.

3.1 3D spherically harmonic trap ($\lambda \equiv 1$)

For a 3D trap with spherical symmetric potential $U(\mathbf{r}) = M\omega_\perp^2 r^2/2$, we suppose that the quantum numbers n_r, l, m make sense in the many-body system at finite N since $n = \{n_r, l, m\}$ present the complete set of the modes. Choosing the excitation operator $f(\mathbf{r}) = r^a Y_{lm}(\theta, \varphi)$ with $a = 2n_r + l$ and Y_{lm} the spherical harmonics and using $\nabla^2 f = n_2 f/r^2$

with $n_2 = 2n_r(2n_r + 2l + 1)$, we get from equations (3), (5) and (6) the results

$$S_1 = \frac{\hbar^2}{4M} [a^2 + l(l+1)] \langle r^{2a-2} \rangle_0, \quad S_U = \hbar^2 \omega_\perp^2 a S_1, \quad (9)$$

$$S_V = \frac{\hbar^4}{4M^2} a(2a-1)n_2 V_V \quad (10)$$

with $V_V = \langle g\delta(\mathbf{r} - \mathbf{r}')r^{2a-4} \rangle'_0$. The choice of the form $Y_{lm}(\theta, \varphi)$ in $f(\mathbf{r})$ comes from the nature of the eigenstates in two limits of $N = 1$ and $N \rightarrow \infty$. When the excitation operators $Y_{lm}(\theta, \varphi)$ are taken in the exact ground state at finite N , it still is an eigenstate of the system in 2D angular coordinates (θ, φ) . The system has the spherical symmetry at finite particle numbers for the entire modes. Taking advantage of this symmetry one needs only to consider the radial part of the ground-state wave function $|N\rangle_0$ since the expectation values taken in $|N\rangle_0$ in separated variables (θ, φ) have been carried out easily below. Thus the calculation of S_1 and S_3 have been greatly simplified. The choice of the form r^a in $f(\mathbf{r})$ comes from the nature of the density fluctuations of the entire modes (n_r, l modes). r^a is a leading term of the radial series solutions of the Schrödinger equation and Gross-Pitaevskii equation at $N = 1$ and $N \rightarrow \infty$, respectively, focusing on exciting the chosen n_r, l mode generally. If we choose f as the a th order polynomial, the sum-rule estimate is wrong even if with and without the correction of S_T since the f excites a lot of other noninteracting states. The lower-order terms in f excite a lot of lower levels, leading the spectral density to be smooth. Carrying out the algebra in equation (7) carefully, the terms higher than second-order partial differentiations have been canceled each other, there only keep down three terms

$$S_T = \frac{-\hbar^6}{2M^3} a(a-1) [a^2 + l(l+1)] \times \left\langle r^{2a-4} \left\{ \frac{\partial^2}{\partial r^2} + \frac{2}{r}(a-1)\frac{\partial}{\partial r} + \gamma \frac{n_2}{r^2} \right\} \right\rangle_0, \quad (11)$$

with $a \geq 1$. The second-order and first-order differentiation terms come from the Laplacian of the kinetic energy. Where γ is a quantum-number-dependent nonzero constant, presenting the non-quantum background. It is not worthwhile to write the formula of γ in more detail since the shift correction is equivalent to set $\gamma = 0$ for reflecting the quantum fluctuations only. Quantum effects original from the fluctuations which behave as the gradient operator rather than the constant operator taken in the ground state. In other words, the reserved part in S_T just is the corrected $S_T^c = S_T - \delta S_T$ by letting $\gamma = 0$ in equation (11), a true kinetic energy contribution to S_3 . It is shown from equation (11) that S_T^c originals from the quantum fluctuations of the ground-state wave function, and that $\delta S_T \propto \gamma$, the shift of S_T , comes from the background of the ground-state wave function. By shifting this background, the peak positions of the spectral density will be at $\omega = \omega_n$. The scheme works well and equation (8) is useful for finite N for the entire modes. In some special symmetric modes,

such as in the surface modes $0l$ where n_2 in per-factor of γ vanishes due to $\nabla^2 f = 0$, $\delta S_T \propto n_2 \gamma = 0$ and the usual sum-rule approaches are correct [4]. In most symmetric modes, however, we need the shift correction.

We now calculate and correct S_V in equation (10). The interaction virial $V_V = \langle g\delta(\mathbf{r} - \mathbf{r}')r^{2a-4} \rangle'_0$ is a two-fold integral, the generalized virial identity can reduce it to two one-fold integrals. Substituting equation (36) into equation (10), we get the simple result $S_V = (\hbar^4/2M^2)an_2(V_U - V_T)$. The correction factor β is determined by the value of $\tilde{\omega}_{n_r,l}^2(\infty)$. This enhancement factor of the collective interaction is

$$\beta = \beta_{n_r,l} = n_r + \frac{l}{2} + \frac{l(l+1)}{2(2n_r+l)}. \quad (12)$$

In some lowest excited states, it needs not to correct S_V [4,18]: for the surface modes $0l$, $S_V = 0$ for $\nabla^2 f = 0$; for the lowest monopole mode 10 , $\beta = 1$ in equation (12). In general $\beta \neq 1$, the correction is necessary.

Substituting equations (10–12) into equation (8), the general EES for the trap with spherically harmonic symmetry is expressed analytically as

$$\tilde{\omega}_{n_r,l}^2(N) = a + \frac{1}{2}n_2 - n_2 \frac{V_T}{2V_U} + a(a-1) \frac{V_T^c}{V_U}, \quad (13)$$

where $V_T^c = -(\hbar^2/2M)\langle r^{2a-4}\partial^2/\partial r^2 + 2(a-1)r^{2a-5}\partial/\partial r \rangle_0$ is the kinetic energy virial. Equation (13) gives all EES information for the entire modes $n_r l$ as long as we have the knowledge of the ground state in the N -body system. Specially at $N = 1$, the eigenfunction $|1\rangle_0$ is exactly Gaussian, we have $V_T = V_T^c = V_U$. From equation (13), $\tilde{\omega}_{n_r,l}(1) = a = 2n_r + l$, just an exact eigenvalue after a good choice of f and a correct shift correction on S_T . At the opposite limit of $N \rightarrow \infty$, $V_T = V_T^c \rightarrow 0$, equation (13) gives $\tilde{\omega}_{n_r,l}^2(\infty) = a + n_2/2 = 2n_r^2 + 2n_r l + 3n_r + l$, just a correct EES after a good choice of f and a correct factor correction on S_V . Therefore, by the aid of the control theory for the asymptotic behavior and the corrected sum-rule estimates, equation (13) in whole middle ranges is available when the ground-state wave function is well defined.

Unfortunately, by now we don't have the exactly analytic expression for the ground-state wave function $|N\rangle_0$ in 3D interacting N -body Bose gases with the harmonic traps. Although the self-consistent wave function $|N\rangle_0$ is readily calculated numerically [11–16], it is often useful to apply an analytic approximation to equation (13) for getting an explicit analytic formula. A boundary-layer formalism [20] solved the kinetic energy divergence problem in the Thomas-Fermi limit. Two very different approximations have been proposed [21]: a Gaussian trial function in small N regime and a Thomas-Fermi approximation in large N limit. A multi-parameter variational trial function [22] has already been found. This function includes the Gaussian function in small N limit, approaches the correct Thomas-Fermi result in large N limit and yields an interpolation for intermediate values of N . For simplicity, we next consider a Gaussian approximation and use variational method in order to calculate equation (13)

explicitly. The EES of equation (13) for all modes $n_r l$ simplifies to [18]

$$\begin{aligned} \tilde{\omega}_{n_r,l}^2(N) &= (2n_r + l)^2 q^2 + (2n_r^2 + 2n_r l + 3n_r + l)(1 - q^2) \\ &= \tilde{\omega}_{n_r,l}^2(1)q^2 + \tilde{\omega}_{n_r,l}^2(\infty)(1 - q^2), \end{aligned} \quad (14)$$

a linear combination with the probabilities q^2 at $N = 1$ and $1 - q^2$ at $N \rightarrow \infty$. This result is valid for the whole parameter ranges of $N[1, \infty)$, $p[0, \infty)$ and corresponding $q[1, 0)$. Where q is a function of the variable $p = \sqrt{2/\pi}(a_{sc}/a_{ho})(N - 1)$ by $p = (1 - q^2)/2q^{5/2}$. Actually, it is very simple to use q as a variable in the range of $q(0, 1]$. Although the Gaussian approximation is not a Thomas-Fermi form, both the controlling of the asymptotic behavior for $\omega_{n_r,l}(N)$ and the variation parameter behavior of $q \rightarrow 0$ at $N \rightarrow \infty$ ensures that equation (14) has a correct result in Thomas-Fermi limit. Equation (14) shows that the EES for all modes has the decrease behavior with increasing the parameter p , except for the surface excitation mode 10 , $\tilde{\omega}_{10}^2(N) = 5 - q^2$, which shows an increase behavior. This predication is consistent with the numeral results [11,12]. However, the result of 20 mode in [12] is not obey equation (14) in that its value in the $N \rightarrow \infty$ limit is higher than the $N = 1$ value. From (14) we have $\tilde{\omega}_{20}^2(N) = 14 + 2q^2$. At $N = 1$, $q = 1$ and $\tilde{\omega}_{20}(1) = 4$; while at $N \rightarrow \infty$, $q = 0$ and $\tilde{\omega}_{20}(\infty) = \sqrt{14} < 4$. The variation parameter q decreases monotonically with the increase of N , in that case the behavior of 20 mode shown in the figure in [12] would indeed be wrong. The result of equation (14) is also valid for the negative scattering length ($a_{sc} < 0$). With increasing values of $-p$, the attractive interaction becomes more and more important, up to the point, $-p_c$, where an unstable condensate forms that would collapse. From the condition $\tilde{\omega}_{10}(N_c) = 0$ and the equation $-p_c = (1 - q_c^2)/2q_c^{5/2}$, one has the critical point at $q_c = \sqrt{5}$ and $p_c = -2/5^{5/4}$. Hence, in that case the collapse region is in $q(1, q_c)$ and $p(p_c, 0)$. Except for the soft of the 10 mode (the soft of the 01 mode doesn't appear in the sum-rule approaches), the entire modes are hard in the collapse region. Figure 1 shows some of the lowest elementary excitation spectra in both regions.

To compare our results with numerical points presented in [15] for an isotropic harmonic trap ($\lambda = 1$), one takes the same parameters for Cs atoms contained in the trap of $\nu_{\perp} \equiv \omega_{\perp} = 10$ Hz. These values of the parameters are $M = 2.2 \times 10^{-25}$ kg, $a_{sc} = 3.18$ nm, $g = 2.0 \times 10^{-51}$ Jm³, $a_{ho} = 1.95\sqrt{2} \times 10^{-6}$ m and $N = 10546$. The value of p then becomes $p = 9.70207$ and the solution of q^2 is $q^2 = 0.086729$. Table 1 presents the comparison for some low-lying modes. Our computation $\tilde{\omega}^{srv}$ comes from equation (14) and numerical points $\tilde{\omega}^{num}$ adopt from Tables I and II of [15] with a maximum basis-set size $N_{basis} = 40$. The difference between $\tilde{\omega}^{num}$ and $\tilde{\omega}^{srv}$ ranges from 0% to 19%. The numerical differences come both from the Gaussian approximation of $|N\rangle_0$ and from the hydrodynamic approximation for bigger quantum numbers.

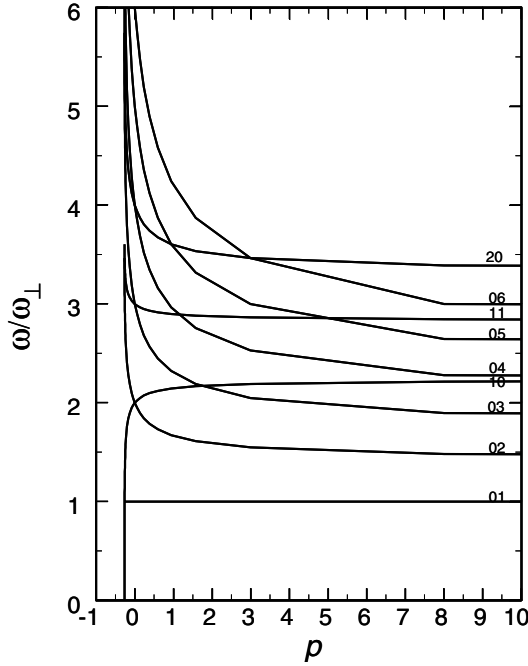


Fig. 1. The elementary excitation spectra as a function of the interaction strength parameter p , including the negative scattering length, for different $n_r l$ modes in the spherically symmetric harmonic potential traps ($\lambda \equiv 1$).

3.2 2D circularly harmonic trap ($\lambda \equiv 0$)

We assume that the chosen quantum numbers $n = \{n_s, m\}$ are available since the radial parity $P_s = [+]$ is alive and $P_s = [-]$ is forbidden at finite N . We now choose in general the excitation operator as $f(\mathbf{r}) = s^b \exp(im\varphi)$ with $b = 2n_s + |m|$ since $\exp(im\varphi)|N\rangle_0$ is still an eigenstate in the expectation-value calculations of S_1 and S_3 and s^b is a leading term of the radial series solutions of the Schrödinger equation and Gross-Pitaevskii equation at $N = 1$ and $N \rightarrow \infty$. From equations (3), (5) and (6) we get

$$S_1 = \frac{\hbar^2}{2M} \langle (b^2 + m^2) s^{2b-2} \rangle_0, \quad S_U = \hbar^2 \omega_\perp^2 b S_1, \quad (15)$$

$$S_V = \frac{\hbar^4}{M^2} b(b-1)(b^2 - m^2) \langle g\delta(\mathbf{s} - \mathbf{s}') s^{2b-4} \rangle'_0. \quad (16)$$

From equation (37) then equation (16) turns to

$$S_V = \frac{\hbar^4 \omega_\perp^2}{M} \frac{b(b-1)(b^2 - m^2)}{2b-1} \left[\langle s^{2b-2} \rangle_0 + a_{\text{ho}}^4 \left\langle (2b-3)s^{2b-4} \frac{\partial^2}{\partial s^2} + (2b^2 - 6b + 5) s^{2b-5} \frac{\partial}{\partial s} \right\rangle_0 \right]. \quad (17)$$

In the limit $N \rightarrow \infty$, we neglect the kinetic energy with respect to the interatomic interaction, i.e., vanishing the partial differentiations in equation (17). From $\tilde{\omega}_{n_s m}^2(\infty) = b + (b^2 - m^2)/2$ [5] and $S_T^c \rightarrow 0$ in equation (8), we find that the correction factor β is expressed

Table 1. A comparison of the numerical data in [15] for a maximum basis-set size $N_{\text{basis}} = 40$ with a calculation of equation (14) using the same parameters of $a_{\text{sc}} = 3.18$ nm, $a_{\text{ho}} = 1.95\sqrt{2} \times 10^{-6}$ m and $N = 10546$.

$n_r l$	$\tilde{\omega}^{\text{num}}$	$\tilde{\omega}^{\text{srv}}$	% diff.
01	1.000	1.000	0.00
02	1.562	1.474	3.53
03	2.065	1.876	10.1
10	2.193	2.217	1.08
04	2.660	2.245	18.5
11	2.872	2.844	0.98
12	3.510	3.381	3.82
20	3.872	3.765	2.84
13	4.156	3.867	7.47
21	4.636	4.418	5.09
14	4.828	4.318	11.8
22	5.373	5.004	7.37
30	5.598	5.271	6.21
23	6.104	5.544	10.1
31	6.422	5.942	8.42
24	6.844	6.050	13.1
32	7.223	6.557	10.2
40	7.383	6.763	9.17
90	16.76	14.17	18.3

exactly for the $n_s m$ modes as

$$\beta_{n_s m} = \frac{(2b-1)(b^2 + m^2)}{4b(b-1)}. \quad (18)$$

This is an enhancement factor due to the collective interaction effects. From equation (7) it is easy to deduce

$$S_T^c = \frac{-\hbar^6}{2M^3} b(b-1)(b^2 + m^2) \times \left\langle s^{2b-4} \frac{\partial^2}{\partial s^2} + (2b-3)s^{2b-5} \frac{\partial}{\partial s} \right\rangle_0. \quad (19)$$

Where we have shifted the constant operator γ terms with respect to the differentiation terms and used the independence of the ground-state wave function on the polar angle φ . Consequently, from equation (8) the analytic expression for the EES is

$$\tilde{\omega}_{n_s m}^2(N) = b - b(b-1) \frac{a_{\text{ho}}^4}{\langle s^{2b-2} \rangle_0} \times \left\langle s^{2b-4} \frac{\partial^2}{\partial s^2} + (2b-3)s^{2b-5} \frac{\partial}{\partial s} \right\rangle_0 + \frac{1}{2} (b^2 - m^2) \left[1 + \frac{a_{\text{ho}}^4}{\langle s^{2b-2} \rangle_0} \times \left\langle (2b-3)s^{2b-4} \frac{\partial^2}{\partial s^2} + (2b^2 - 6b + 5) s^{2b-5} \frac{\partial}{\partial s} \right\rangle_0 \right]. \quad (20)$$

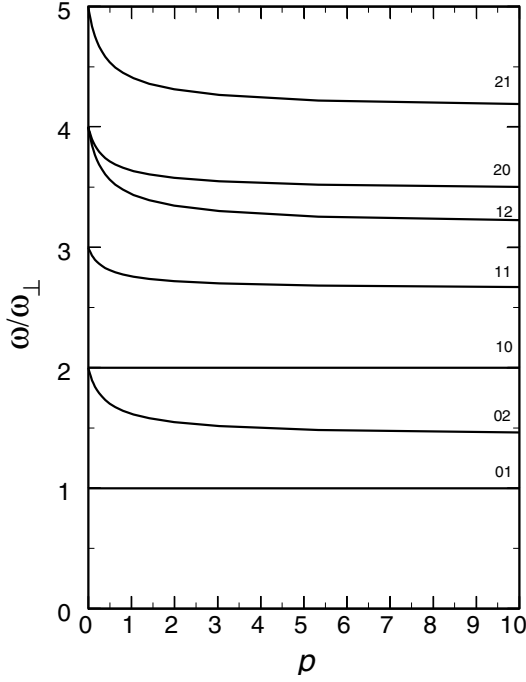


Fig. 2. The elementary excitation spectra as a function of the interaction parameter p for different $n_s m$ modes in the circularly symmetric harmonic potential traps ($\lambda \equiv 0$).

This is an important result that includes obviously the two limiting cases $\tilde{\omega}_{n_s m}(1) = b$ and $\tilde{\omega}_{n_s m}^2(\infty) = b + (b^2 - m^2)/2$ and yields reasonably a useful interpolation.

In a variational Gaussian calculation, the trial ground-state wave function with a single variation parameter q takes the form $|N\rangle_0 = (\sqrt{N}/a_{\text{ho}})(q/\pi)^{1/2} \exp(-q\tilde{s}^2/2)$ with $\tilde{s} = s/a_{\text{ho}}$. From equation (1) we calculate the expectation value of the ground-state energy as $E_0 = \hbar\omega_{\perp}(\frac{1}{q} + q + 2pq^{3/2})/2$. From $\partial E_0/\partial q = 0$, q is the positive real root of the equation $1 - q^2 = 3pq^{5/2}$. Thus the EES for all modes $n_s m$ is expressed explicitly as

$$\tilde{\omega}_{n_s m}^2(N) = b + \frac{1}{2}(b^2 - m^2) + \frac{1}{2}(b^2 - 2b + m^2)q^2. \quad (21)$$

This result is also valid for the whole parameter ranges of $N[1, \infty)$, $p[0, \infty)$ and $q[1, 0)$, and shows clearly a linear combination of $\tilde{\omega}_{n_s m}^2(1)$ and $\tilde{\omega}_{n_s m}^2(\infty)$ with the probabilities q^2 and $1 - q^2$: $\tilde{\omega}_{n_s m}^2(N) = \tilde{\omega}_{n_s m}^2(1)q^2 + \tilde{\omega}_{n_s m}^2(\infty)(1 - q^2)$. Figure 2 shows the plots of $\omega_{n_s m}/\omega_{\perp}$ versus p for different $n_s m$ modes in the traps ($\lambda \equiv 0$) with the circular symmetry.

3.3 3D cylindrically harmonic trap ($\lambda \neq 1$)

By extending the 2D excitation operator, we choose in general $f(\mathbf{r}) = s^b z^k \exp(im\varphi)$ with $k = \alpha n_z$. In the choice of the excitation operators in single-body 1D axial, many-body 3D spherical and 2D circular symmetries of the harmonic oscillators we remember that the radial operators x^n , r^a and s^b are all the leading terms of the radial series

solutions of the Schrödinger equation and Gross-Pitaevskii equation at $N = 1$ and $N \rightarrow \infty$, if one needs to excite modes $n = \{n\}$, $\{n_r, l, m\}$ and $\{n_s, m\}$, respectively. These simple choices lead equation (8) to have exact results at $N = 1$ after shifting the non-quantum background in the spectral density of S_T . Another choices of the excitation operator make a vain attempt, not only creating a lot of new crossing terms, but also exciting a lot of other noninteracting levels. However, the existence of the coupling between s and z is an innate character for the cylindrically symmetrical system. For simplicity, we choose the coupled leading term as $s^b z^k$ and introduce a parameter $\alpha \neq 1$ to represent the coupling between the axial and radial motions. From equations (3), (5) and (6) we get

$$\begin{aligned} S_1 &= \frac{\hbar^2}{2M} \left\langle (b^2 + m^2) s^{2b-2} z^{2k} + k^2 s^{2b} z^{2k-2} \right\rangle_0, \\ S_U &= \hbar^2 \omega_{\perp}^2 (b + \lambda^2 k) S_1, \\ S_V &= \frac{\hbar^4}{2M^2} \left\langle g\delta(\mathbf{r} - \mathbf{r}') \left\{ 2b(b-1)(b^2 - m^2) s^{2b-4} z^{2k} \right. \right. \\ &\quad \left. \left. + k(4b^2 k - 3b^2 - 2km^2 + m^2) s^{2b-2} z^{2k-2} \right. \right. \\ &\quad \left. \left. + k^2(k-1)(2k-3) s^{2b} z^{2k-4} \right\} \right\rangle_0'. \end{aligned} \quad (22)$$

In order to reduce the two-fold integral in equation (23) into the one-fold integrals, we generalize the virial identity (37) to the case of the axial symmetry (see Appendix B). By the use of equation (38) with the different values of μ and ν , equation (23) in the one-fold integral reads to equation (39) in Appendix C.

The calculation of S_T in equation (7) is very complicated. After some lengthy, but straight forward algebra very carefully, we find a general expression for S_T^c entering in equation (40) in Appendix C. Here we have shifted the constant operator γ terms and used the independence of the ground-state wave function on the polar angle φ , as well as arrived the result that the terms higher than two-order partial differentiations have been canceled each other in the commutator calculations. The over length expressions for S_V and S_T^c in equations (39) and (40) come from two variables s and z and their coupling. In the limit of $N \rightarrow \infty$, $S_T^c \rightarrow 0$ and the kinetic energy contribution to S_V vanishes. The correction factor β is determined entering in equation (39) of Appendix C. It is not necessary to make this correction factor for some modes with $\nabla^2 f = 0$ in which $S_V = 0$ already; the parameter α will be determined below for the strong coupling modes, while for the decoupling modes with $n_s = 0$, one has $\alpha = 1$ and with $n_z = 0$ one has $k = 0$.

Consequently, from equation (8) the analytic expression for the EES with the cylindrically harmonic trap is

$$\tilde{\omega}_{n_z n_s m}^2(N) = b + \lambda^2 k + (S_T^c + \beta_{n_z n_s m} S_V)/\hbar^2 \omega_{\perp}^2 S_1. \quad (24)$$

This is our key result. Here S_1 , S_V and S_T^c are expressed in equations (22), (39) and (40), respectively. The factor $\beta_{n_z n_s m}$ is expressed in equation (41) and the coupling parameter α , appearing in $k = \alpha n_z$, will be determined by the condition of $\tilde{\omega}_{n_z n_s m}(1) = 2n_s + |m| + \lambda n_z$.

$$\begin{aligned}
\tilde{\omega}_{110}^2(N) = & 2 + \lambda^2\alpha + \frac{q^2}{2\alpha - 1 + \tilde{\lambda}\alpha^2} \left[2(2\alpha - 1) + 2\alpha(5\alpha - 1)\tilde{\lambda} + \alpha(6\alpha^2 - 3\alpha - 1)\tilde{\lambda}^2 + \alpha^3(\alpha - 1)\tilde{\lambda}^3 \right] \\
& + \frac{\beta_{110}}{(2\alpha + 3)(2\alpha - 1 + \tilde{\lambda}\alpha^2)} \left\{ 2(4\alpha^2 - 1)\lambda^2/\tilde{\lambda} + (2\alpha - 1)[4 + \alpha(4\alpha - 3)\lambda^2] + \alpha[4(4\alpha - 3) + \alpha(\alpha - 1)(2\alpha - 3)\lambda^2]\tilde{\lambda} \right. \\
& \left. + 6\alpha^2(\alpha - 1)\tilde{\lambda}^2 - q^2[4(2\alpha - 1) + 2(12\alpha^2 - 6\alpha - 1)\tilde{\lambda} + \alpha(14\alpha^2 - 16\alpha + 3)\tilde{\lambda}^2 + \alpha^2(\alpha - 1)(2\alpha - 3)\tilde{\lambda}^3] \right\} \quad (27)
\end{aligned}$$

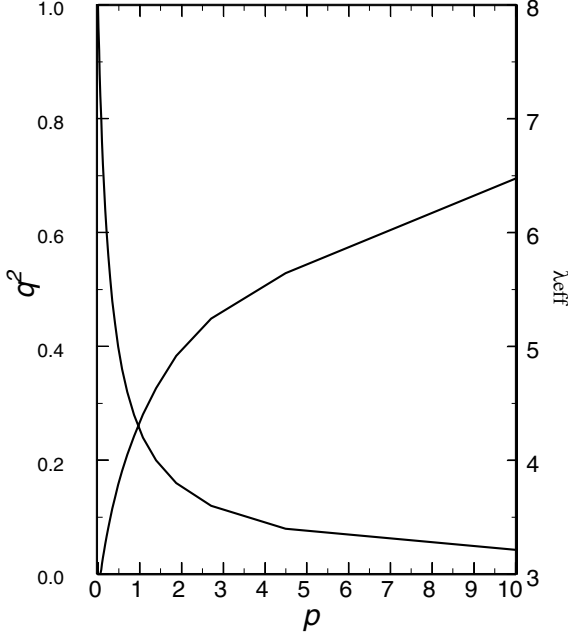


Fig. 3. The variational parameters as a function of the interaction strength p in the axially symmetric harmonic potential traps with $\lambda = \sqrt{8}$. The left vertical axis is the “single-body probability” q^2 and the right vertical axis is the effective-frequency ratio $\lambda_{\text{eff}} = \tilde{\lambda}$.

For getting the explicit expressions for $\tilde{\omega}_{n_z n_s m}(N)$, we use the simple variational Gaussian ground-state wave function in the N -body system by introducing two variation parameters q and $\tilde{\lambda}$ [18]. Figure 3 shows the plots of q^2 (left vertical axis) and $\tilde{\lambda} = \lambda_{\text{eff}}$ (right vertical axis) versus p with $\lambda = \sqrt{8}$. The “single-body probability” $q^2 - \tilde{\omega}_{n_z n_s m}^2(1)$ contribution to $\tilde{\omega}_{n_z n_s m}^2(N)$, decreases sharply with increasing of p in small N regime. The many-body effects dominate the dynamics of the system in large N regime. The explicit expression for the EES is

$$\begin{aligned}
\tilde{\omega}_{n_z n_s m}^2(N) = & b + \lambda^2 k \\
& + \frac{\xi q^2 + \beta_{n_z n_s m}(\eta - \zeta q^2)/(2k + 2b - 1)}{(2k - 1)(b^2 + m^2) + 2k^2 b \tilde{\lambda}}. \quad (25)
\end{aligned}$$

The quantities entering in equation (25) are defined in equations (42–44).

It is easy to show that for $q \rightarrow 0$, $p \rightarrow \infty$ and $\tilde{\lambda} = \lambda^2$ at $N \rightarrow \infty$, the final result of equation (25) turns to the result of equation (42), and that for $q = 1, p = 0$

and $\tilde{\lambda} = \lambda$ at $N = 1$, the interaction energy contribution to $\tilde{\omega}_{n_z n_s m}^2(N)$ in equation (42) vanishes. This check proves our correct calculations. In the absence of the interatomic interaction, substituting $\tilde{\omega}_{n_z n_s m}(1) = b + \lambda n_z$, $q = 1$ and $\tilde{\lambda} = \lambda$ at $N = 1$ into equation (42), we find that α is the positive real root of the algebra equation

$$\begin{aligned}
[(b + \lambda n_z)^2 - (b + \lambda^2 k)] [(b^2 + m^2) + (2k - 1) + 2b\lambda k^2] = \\
b(b - 1)(b^2 - m^2)(2k - 1) + 2\lambda [b(3b^2 k - bk - b^2 + b) \\
+ (b - 1)m^2(2k - 1)]k + [6k^2 - 3k - 1]b^2 \\
+ m^2(k + 1)(2k - 1)\lambda^2 k + 2b\lambda^3 k^3(k - 1). \quad (26)
\end{aligned}$$

In fact, we only need to choose the root near 1. $\alpha \gtrsim 1$ for $\lambda > 1$ and $\alpha \lesssim 1$ for $\lambda < 1$. Of course, $k = 0$ for $0n_s m$ modes and $k = 1$ for $n_z 00$ and $10m$ modes. They are decoupling modes and hence they recover the harmonic oscillator results of $\tilde{\omega}_{n_z n_s m}(1) = \lambda n_z + 2n_s + |m|$ in the absence of the interatomic interaction. There is neither shift correction on S_T nor factor correction on S_V for the $00m$ and $10m$ modes with $m = 0, \pm 1, \pm 2, \dots$. For the $0n_s 0$ and $n_z 00$ modes the multiplicative factor is necessary for correcting S_V with $n_s \geq 1$ and $n_z \geq 2$ and the shift is necessary for correcting S_T with $n_s \geq 2$ and $n_z \geq 3$. For these decoupling modes, after the suitable choice of f and correct shift correction on S_T , the results of equation (24) are exact at $N = 1$ since the state $|1\rangle_0$ is exact. We can't get the given $\tilde{\omega}_{n_z n_s m}(1) = b + \lambda n_z$ directly from equation (24) for the coupling modes, even if with another choices of f and another corrections on S_T . As mentioned above, in that wrong way it is impossible to get the correct result of $\tilde{\omega}_{n_z n_s m}(1)$. We insistently use this physical correction and extend the choice of f to the coupling modes by introducing the parameter α . Furthermore we use $\tilde{\omega}_{n_z n_s m}(1) = b + \lambda n_z$ as a known boundary condition to determine α in equations (24) or (25).

To illustrate the properties of the EES we write out several typical results explicitly. From equations (25) and (26) we have $\tilde{\omega}_{001}^2(N) = 1$, $\tilde{\omega}_{002}^2(N) = 2(1 + q^2)$, $\tilde{\omega}_{010}^2(N) = 2 + 2q^2 + 2\beta_{010}[2 + \lambda^2/\tilde{\lambda} - (2 + \tilde{\lambda})q^2]/3$, $\tilde{\omega}_{100}^2(N) = \lambda^2$, $\tilde{\omega}_{101}^2(N) = 1 + \lambda^2 + 2\tilde{\lambda}q^2$ and

see equation (27) above.

Where $\alpha = \alpha_{110}$ satisfies equation (26) which simplifies to

$$\lambda^2 \alpha^4 + 6\lambda \alpha^3 + (8 - 5\lambda - \lambda^2) \alpha^2 - 2(5 + 2\lambda)\alpha + 4 + \lambda = 0. \quad (28)$$

Figure 4 shows the plots of $\omega_{n_z n_s m}/\omega_{\perp}$ versus p for those modes with $\lambda = \sqrt{8}$ in the axially symmetrical trap. The

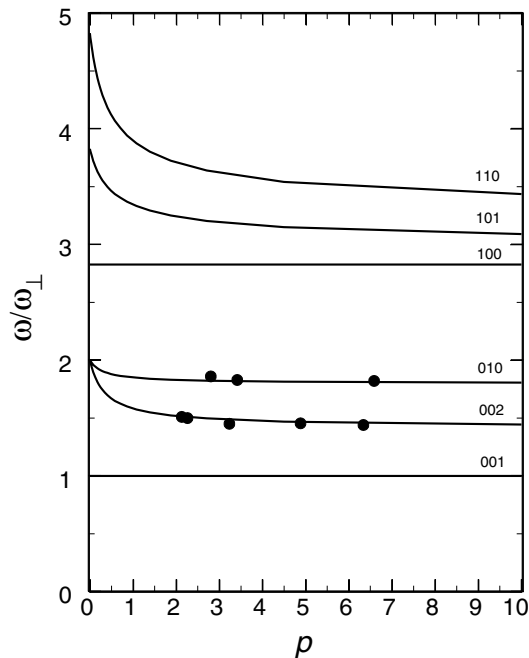


Fig. 4. The elementary excitation spectrum as a function of the interaction parameter p for different $n_z n_s m$ modes in the axially symmetric harmonic potential traps with $\lambda = \sqrt{8}$. The dots represent experimental data for 002 and 010 modes with $\lambda = \sqrt{8}$ [23].

results agree well with the experimental data [23] denoted by the dots for 002 and 010 modes. These two modes have the boundary values $\tilde{\omega}_{002}(1) = \tilde{\omega}_{010}(1) = 2$ at $N = 1$ and $\tilde{\omega}_{002}(\infty) = \sqrt{2}$ and $\tilde{\omega}_{010}(\infty) = \sqrt{14 - \sqrt{116}} \simeq 1.79713$ at $N \rightarrow \infty$. And hence one finds $\beta_{010} = [\tilde{\omega}_{010}^2(\infty)/2 - 1] \simeq 0.614835 < 1$, leading $\tilde{\omega}_{010}(N)$ to be lower than the upper boundary estimate of the usual sum-rule approaches. From equation (28) we solve $\alpha_{110} = 1.08871$ for $\lambda = \sqrt{8}$, representing the coupling between the z - and s -direction motions.

We have compared our results with experimental data [23] and numerical points [11]. The frequency ratio is taken to be $\lambda = \sqrt{8}$ and the scattering length is taken to be $a_{sc} = 110$ a.u. = 5.82 nm. For given values of z -axis frequency ν_{\perp} and condensate-number parameters N , we calculated the harmonic-oscillator length scale a_{ho} and the interaction parameter p . From equation (25) we calculated the values of $\tilde{\omega}_{n_z n_s m}^2(N)$. The comparison is shown in Table 2. The experimental [23] and numerical [11] data adopt from Table 1 of [11] and the modes mark in our notation. It is shown that the agreement is excellent and the difference between theory and experiment ranges from 1% to 5%.

4 Summary and discussion

The combination of the corrected sum rules and generalized virial identities has been used to calculate analytically the elementary excitation spectrum for the entire

Table 2. A comparison of the data of [11] with a calculation of equation (25) using the actual experimental trap ($\lambda = \sqrt{8}$, $a_{ho} = 3.32 \times 10^{-6}$ m for $\nu_{\perp} \equiv \omega_{\perp}/2\pi = 132$ Hz), scattering-length ($a_{sc} = 110$ a.u.), and condensate-number parameters (N) of [23].

$n_z n_s m$	ν_{\perp}	N	$\tilde{\omega}^{\text{exp}}$	$\tilde{\omega}^{\text{num}}$	$\tilde{\omega}^{\text{srv}}$	% ^{num}	% ^{srv}
002	132	2200	1.39–1.42	1.47	1.46	5.8	5.0
002	43.2	2800	1.41–1.44	1.49	1.48	5.7	5.0
010	132	2400	1.79–1.83	1.88	1.81	5.0	1.1
010	43.2	3420	1.84–1.88	1.89	1.81	2.7	1.6

modes of interacting gases of finite bosons in harmonic traps with 3D spherical symmetry, 2D circular symmetry and 3D axially anisotropic symmetry. We have chosen the leading term of the radial series solutions of the nonlinear Schrödinger equation as the radial excitation operator and used the eigenfunctions in other motion directions due to the symmetries. We have extended the form of the excitation operator for some low-lying modes to the entire modes with certain kind of symmetries and corresponding quantum numbers. Along this line we have taken the corrections of the cubic sum rules for having the sharp peak positions of the spectral density in sum rules S_1 and S_3 . According to the control theory for the asymptotic behavior, we have determined uniquely the corrections of cubic sum rules both in kinetic energy constant shift and in potential energy multiplicative factor for all modes, and hence the calculations are true as long as we know the N -body ground state. By the use of the generalized virial identities, we have reduced the calculation associated with the interaction energy from a two-fold integral to two one-fold integrals, and hence the cubic sum rule of the interaction energy is expressed by those of potential and kinetic energies. We have obtained the explicit analytic expressions for the entire energy spectra by using the simple variational Gaussian ground-state wave function of the N -body condensate in the traps with spherically, circularly and axially symmetric harmonic-oscillator potentials. We have also obtained the dependence of the entire energy spectra on the atom number in the trap and on the interatomic interaction strength, as well as on the trap geometry parameter. There are not any variable control parameters in the formulas for the elementary excitation spectrum. Our results are illustrated in Figures 1–4 and the comparison is summarized in Tables 1 and 2. The previous analytic and numerical results are only some special cases for the low-lying excitation modes.

The choice of the form of excitation operator in this work is simplest and useful by taking advantage of the symmetries of the system under consideration. The calculations of S_1 and S_3 have been greatly simplified by taking account of the radial part of the ground-state wave function only. As the radial excitation operator, it is impossible to choose the linear combination of some lower terms in the radial series solutions of the nonlinear Schrödinger equation since these terms excite a lot of other noninteracting states. After this best choice of f , one needs to

correct the cubic sum rules S_T and S_V associated with the kinetic and potential energies. The shift correction on S_T , determined by the boundary value $\omega_n(1)$, means to drop the constant spectral density in order to appear the quantum fluctuation effects. The factor correction on S_V , determined by the boundary value $\omega_n(\infty)$, controls the magnitude of the elementary excitation spectrum in the whole range of p . The quantum corrections on $\omega_n(\infty)$ [7] do not change the analytic formulas, but improve the magnitudes in the whole range of q as well as p . Specifically for the higher-lying excitation modes, the numerical solution $\omega_n(\infty)$ of the Bogoliubov equations improves the magnitudes significantly. The calculation of the elementary excitation spectrum is valid for whole range from small to large atom numbers. For the higher energy levels with the strong coupling between the axial and radial motions, the introduced parameter α is determined by the boundary condition of $\omega_n(1)$. It is worthwhile to point out that we have obtained the explicit analytic expression for $\omega_{n_z n_s m}(N)$. Funnily the limiting result $\omega_{n_z n_s m}(\infty)$ doesn't still have the explicit analytic expression. For all modes the hydrodynamic results in the strong interaction case have been known as a boundary condition. Therefore, the explicit analytic results in the middle ranges are available and the analytic expressions for the entire energy spectrum provide enough information for the quantum statistics of the N -body nonhomogeneous interacting Bose gases. Since the elementary excitation concept presented by Landau has the strongest physical intuition and the measurement of energy spectrum of these elementary excitations has the finest precision, we suggest that the further experiments and numerical works consider the higher excitation states to confirm our predications.

Fetter's trial wave function [22] with three variation parameters maybe are a better choice than ours with two variation parameters. The usual sum-rule approaches combining with Fetter's variational function have obtained the EES of 002 and 010 modes [24]. The plots in Figure 1 of [24] are indistinguishable from our Figure 4. The difference between the Gaussian and Fetter's approximations is very small at small p even at middle p . However, although this difference becomes big at $N \propto p \rightarrow \infty$, the controlling of asymptotic behavior leads the EES to be an given approximative value. Table 1 of [18] has also compared the total energy, kinetic energy, trapping potential energy and interaction energy obtained from the Gaussian approximation with those obtained variationally [22, 24] and numerically [25]. From a practical point of view, it would be interesting to calculate equations (13), (20) and (24) with Fetter's multi-parameter variational functions, but such a calculation remains the finite precision since it has the same value with the variational Gaussian calculation in the limit of infinite bosons [26]. From a theoretical point of view, it is interesting to extend the sum-rule approaches to the Bose-Fermi gas mixture [27], especially generalizing the individual eigenstates [28] to the entire eigenstates.

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Appendix A: Proof of equation (6) the interaction energy contribution to the cubic sum rule

For any V -dependent vector operator $\hat{\mathbf{Q}}(V)$ the Gaussian integral theorem states that

$$\left\langle \left\{ \nabla \cdot \hat{\mathbf{Q}}(V) \right\}' \right\rangle_0 = 0 \quad (29)$$

for $\hat{\mathbf{Q}}(V) = 0$ at the boundary of the system. In fact the interatomic interaction vanishes at the boundary. Along this line the interaction energy functions which arise on commuting with the momentum operator in S_V can be changed to a derivative form in order to avoid the divergence of $\nabla \delta(\mathbf{r})$. We introduce the notation $I = \nabla \cdot (V \nabla f)$ and commutator $J \equiv [(\nabla f^*) \cdot \nabla, (\nabla f) \cdot (\nabla V)] = (\nabla f^*) \cdot (\nabla \{(\nabla f) \cdot (\nabla V)\})$ in S_V . With these notations we find

$$I = (\nabla f) \cdot (\nabla V) + V (\nabla^2 f), \quad (30)$$

$$J = (\nabla f^*) \cdot (\nabla I) - (\nabla f^*) \cdot \{ \nabla [V (\nabla^2 f)] \}. \quad (31)$$

In equation (31), $(\nabla f^*) \cdot (\nabla I) = \nabla \cdot (I \nabla f^*) - I (\nabla^2 f^*)$. Expanding the second term of the right hand of equation (31) and using the complex conjugant of equation (30), one has

$$J = \nabla \cdot (I \nabla f^*) - I (\nabla^2 f^*) - I^* (\nabla^2 f) + V (\nabla^2 f) (\nabla^2 f^*) - V (\nabla f^*) \cdot [\nabla (\nabla^2 f)]. \quad (32)$$

Expanding

$$\nabla \cdot [V (\nabla^2 f) (\nabla f^*)] = (\nabla^2 f) (\nabla f^*) \cdot (\nabla V) + V (\nabla^2 f) (\nabla^2 f^*) + V (\nabla f^*) \cdot [\nabla (\nabla^2 f)]$$

and substituting it into the complex conjugant of equation (30), one has

$$I^* (\nabla^2 f) = \nabla \cdot [V (\nabla^2 f) (\nabla f^*)] - V (\nabla f^*) \cdot [\nabla (\nabla^2 f)]. \quad (33)$$

Substituting equation (33) into its complex conjugant

$$I (\nabla^2 f^*) = \nabla \cdot [V (\nabla^2 f^*) (\nabla f)] - V (\nabla f) \cdot [\nabla (\nabla^2 f^*)]$$

into the equation (32), we finally have

$$J = V \{ (\nabla^2 f) (\nabla^2 f^*) + (\nabla f) \cdot (\nabla \nabla^2 f^*) \} + \nabla \cdot \{ \nabla \cdot (V \nabla f) (\nabla f^*) - V (\nabla^2 f) (\nabla f^*) - V (\nabla^2 f^*) (\nabla f) \}. \quad (34)$$

The expectation value of J in equation (34) gives equation (6) since the operator $\hat{\mathbf{Q}}(V)$ here is the term within the second braces of right hand of equation (34) which vanishes at the boundary.

Appendix B: Generalized virial identities with different symmetric trap potentials

The usual virial identity states that for a system with the form of Hamiltonian $\hat{H} = \sum_{i=1}^N (T + U + V)$, from

$$\begin{aligned}
\langle g\delta(\mathbf{r}-\mathbf{r}')s^\mu z^\nu \rangle'_0 &= \frac{M\omega_\perp^2}{\mu+\nu+3} \langle s^{\mu+2}z^\nu + \lambda^2 s^\mu z^{\nu+2} \rangle_0 \\
&+ \frac{\hbar^2}{2M(\mu+\nu+3)} \left\langle 2(1+\mu)s^\mu z^\nu \frac{\partial^2}{\partial s^2} + \left[(\mu^2+2\mu+2)s^{\mu-1}z^\nu + \nu(\nu-1)s^{\mu+1}z^{\nu-2} \right] \frac{\partial}{\partial s} \right. \\
&\left. + 2\left(\mu s^{\mu-1}z^{\nu+1} + \nu s^{\mu+1}z^{\nu-1} \right) \frac{\partial^2}{\partial s \partial z} + \left[\mu^2 s^{\mu-2}z^{\nu+1} + \nu(\nu+1)s^\mu z^{\nu-1} \right] \frac{\partial}{\partial z} + 2(1+\nu)s^\mu z^\nu \frac{\partial^2}{\partial z^2} \right\rangle_0 \quad (38)
\end{aligned}$$

$\langle dD/dt - \partial D/\partial t \rangle = \langle [D, \hat{H}] \rangle / i\hbar = 0$ at stationary state for a dimensionless operator $D(\mathbf{r}, t) = \mathbf{r} \cdot \nabla$ in the Heisenberg picture, one has the relation among virials

$$\langle \mathbf{r} \cdot \nabla V \rangle = \langle \mathbf{r} \cdot \nabla U \rangle - 2\langle T \rangle. \quad (35)$$

In practice, we need to calculate the expectation value of the weighted interaction energy in equation (6). For doing so we have to introduce a weighted operator D_μ relative to the form of f dependent on the trap symmetries. We will give different moment-weighted virial identities for the corresponding symmetrical potentials.

For a 3D spherically harmonic trap ($\lambda \equiv 1$), we introduce a r^a -weighted operator $D_a = r^a \mathbf{r} \cdot \nabla$ with $a = 2n_r + l$. From $\langle [D_a, \hat{H}] \rangle_0 = 0$ for the stationary state, we have

$$\left(a - \frac{1}{2} \right) V_V = V_U - V_T, \quad (36)$$

where $V_U = \langle M\omega_\perp^2 r^{2a-2}/2 \rangle_0$ is the relative potential virial, $V_T = -(\hbar^2/2M) \langle (2a-3)r^{2a-4} \partial^2/\partial r^2 + (2a^2-5a+4)r^{2a-5} \partial/\partial r \rangle_0$ is the kinetic virial, and all of those are with a moment-weight r^{2a-4} . The weighted virial identity (36) shows that the interaction virial V_V of the two-fold integral is reduced to V_T and V_U of the one-fold integrals. $V_U = V_T$ for $V_V = 0$ without the interatomic interactions.

For a 2D circularly harmonic trap ($\lambda \equiv 0$), we introduce a s^{2b-4} -weighted operator $D_b = s^{2b-4} \mathbf{s} \cdot \nabla$ and generalize the virial identity (36) to the case of the circular symmetry with $b = 2n_s + |m|$. From $\langle [D_b, \hat{H}] \rangle_0 = 0$ for the

stationary state, we find

$$\begin{aligned}
(2b-1) \langle g\delta(\mathbf{s}-\mathbf{r}')s^{2b-4} \rangle'_0 &= M\omega_\perp^2 \langle s^{2b-2} \rangle_0 \\
&+ \frac{\hbar^2}{M} \left\langle (2b-3)s^{2b-4} \frac{\partial^2}{\partial s^2} + (2b^2-6b+5)s^{2b-5} \frac{\partial}{\partial s} \right\rangle_0. \quad (37)
\end{aligned}$$

The interaction virial reduces to the potential virial and relative kinetic virial.

For a 3D cylindrically harmonic trap ($\lambda \neq 1$), we introduce a $s^\mu z^\nu$ -weighted operator $D_{\mu\nu} = s^\mu z^\nu \mathbf{r} \cdot \nabla$ for the different values of μ and ν . From $\langle [D_{\mu\nu}, \hat{H}] \rangle_0 = 0$ for the stationary state, one finds

see equation (38) above.

Obviously, the weighted interaction energy has been expressed as the difference between the weighted external potentials and the kinetic energy in their expectation value (virial) calculations.

Appendix C: General expressions for S_V , S_T^c and $\beta_{n_z n_s m}$ and their Gaussian approximations with $\lambda \neq 1$

After some lengthy, but straight forward algebra by substituting equations (38) and (23) with corresponding values of μ and ν , we have

$$\begin{aligned}
S_V &= \frac{\hbar^4 \omega_\perp^2 / 2M}{2k+2b-1} \left\langle 2b(b-1)(b^2-m^2)\lambda^2 s^{2b-4} z^{2k+2} + \left[2b(b-1)(b^2-m^2) + k(4kb^2-3b^2-2km^2+m^2)\lambda^2 \right] s^{2b-2} z^{2k} \right. \\
&+ k \left[4kb^2-3b^2-2km^2+m^2 + k(k-1)(2k-3)\lambda^2 \right] s^{2b} z^{2k-2} + k^2(k-1)(2k-3) s^{2b+2} z^{2k-4} + a_{\text{ho}}^4 \left\{ \left[2b(b-1)(2b-3)(b^2-m^2) s^{2b-4} z^{2k} \right. \right. \\
&+ k(2b-1)(4kb^2-3b^2-2km^2+m^2) s^{2b-2} z^{2k-2} + k^2(k-1)(2k-3)(2b+1) s^{2b} z^{2k-4} \left. \right] \frac{\partial^2}{\partial s^2} + \left\{ 2b(b-1)(2b^2-6b+5)(b^2-m^2) s^{2b-5} z^{2k} \right. \\
&+ \left[kb^2(12kb^2-12kb-8b^2+8b+4k-3) - k(2k-1)(2b-1)^2 m^2 \right] s^{2b-3} z^{2k-2} + k(k-1)(2k-3)(6kb^2-3b^2+2kb+k \\
&- 2km^2+m^2) s^{2b-1} z^{2k-4} + k^2(k-1)(k-2)(2k-3)(2k-5) s^{2b+1} z^{2k-6} \left. \right\} \frac{\partial}{\partial s} + \left[4b(b-1)(b-2)(b^2-m^2) s^{2b-5} z^{2k+1} \right. \\
&+ 2k(b-1)(4kb^2+2b^3-3b^2-2km^2-2bm^2+m^2) s^{2b-3} z^{2k-1} + 2k(k-1)(2k^2b+4kb^2-3b^2-3kb-2km^2+m^2) s^{2b-1} z^{2k-3} \\
&+ 2k^2(k-1)(k-2)(2k-3) s^{2b+1} z^{2k-5} \left. \right] \frac{\partial^2}{\partial s \partial z} + \left[4b(b-1)(b-2)^2 (b^2-m^2) s^{2b-6} z^{2k+1} + 2k(b-1)(6kb^3-2b^3-4kb^2+3b^2-4kbm^2 \right. \\
&+ 2km^2-m^2) s^{2b-4} z^{2k-1} + k(k-1)(12k^2b^2-16kb^2+3b^2-4k^2m^2+4km^2-m^2) s^{2b-2} z^{2k-3} + k^2(k-1)(k-2)(2k-3)^2 s^{2b} z^{2k-5} \left. \right] \frac{\partial}{\partial z} \\
&+ \left. \left[2(2k+1)b(b-1)(b^2-m^2) s^{2b-4} z^{2k} + k(2k-1)(4kb^2-3b^2-2km^2+m^2) s^{2b-2} z^{2k-2} + k^2(k-1)(2k-3)^2 s^{2b} z^{2k-4} \right] \frac{\partial^2}{\partial z^2} \right\} \right\rangle_0. \quad (39)
\end{aligned}$$

$$\begin{aligned}
S_T^c = & \frac{-\hbar^6}{2M^3} \left\langle \left[b(b-1)(b^2+m^2)s^{2b-4}z^{2k} + k^2b(b+1)s^{2b-2}z^{2k-2} \right] \frac{\partial^2}{\partial s^2} + \left\{ b(b-1)(2b-3)(b^2+m^2)s^{2b-5}z^{2k} \right. \right. \\
& + \left. \left[kb(4kb^2 - kb - k - b^2 + b) + k(2k-1)(b-1)m^2 \right] s^{2b-3}z^{2k-2} + k^2(k-1)(2k-3)bs^{2b-1}z^{2k-4} \right\} \frac{\partial}{\partial s} \\
& + 2k \left[(b-1)(b^2+m^2)s^{2b-3}z^{2k-1} + k(k-1)bs^{2b-1}z^{2k-3} \right] \frac{\partial^2}{\partial s \partial z} + k \left[(k+1)(b^2+m^2)s^{2b-2}z^{2k-2} + k^2(k-1)s^{2b}z^{2k-4} \right] \frac{\partial^2}{\partial z^2} \\
& + 2k \left\{ (b-1)^2(b^2+m^2)s^{2b-4}z^{2k-1} + (k-1) \left[(2k+1)b^2 + (k+1)m^2 \right] s^{2b-2}z^{2k-3} + k^2(k-1)(k-2)s^{2b}z^{2k-5} \right\} \frac{\partial}{\partial z} \Bigg|_0 \quad (40)
\end{aligned}$$

$$\begin{aligned}
\beta_{n_z n_s m} = & \lim_{N \rightarrow \infty} (2k+2b-1) \left[\tilde{\omega}_{n_z n_s m}^2(\infty) - (b+\lambda^2 k) \right] \left\langle (b^2+m^2)s^{2b-2}z^{2k} + k^2s^{2b}z^{2k-2} \right\rangle_0 \langle 2b(b-1)(b^2-m^2)\lambda^2 s^{2b-4}z^{2k+2} \\
& + \left[2b(b-1)(b^2-m^2) + k(4kb^2 - 3b^2 - 2km^2 + m^2)\lambda^2 \right] s^{2b-2}z^{2k} \\
& + k \left[4kb^2 - 3b^2 - 2km^2 + m^2 + k(k-1)(2k-3)\lambda^2 \right] s^{2b}z^{2k-2} + k^2(k-1)(2k-3)s^{2b+2}z^{2k-4} \Bigg|_0^{-1} \quad (41)
\end{aligned}$$

Substituting $f(\mathbf{r}) = s^b z^k \exp(im\varphi)$ into equation (7), we have

see equation (40) above.

Substituting equations (22) and (39) into equation (8) with vanishing of the kinetic energy, for known $\tilde{\omega}_{n_z n_s m}(\infty)$ the correction factor β in general is expressed by

see equation (41) above.

The expressions of equations (39–41) are for the quantities entering in equation (24).

Under the Gaussian approximation, we find the following expressions for the quantities entering in equation (25):

$$\begin{aligned}
\xi \equiv & (2k-1)b(b-1)(b^2+m^2) \\
& + 2k \left[b(3kb^2 - kb - b^2 + b) + (2k-1)(b-1)m^2 \right] \tilde{\lambda} \\
& + k \left[(6k^2 - 3k - 1)b^2 + (k+1)(2k-1)m^2 \right] \tilde{\lambda}^2 \\
& + 2k^3(k-1)b\tilde{\lambda}^3, \quad (42)
\end{aligned}$$

$$\begin{aligned}
\eta \equiv & (4k^2-1)b(b^2-m^2)\frac{\lambda^2}{\tilde{\lambda}} + (2k-1) \left\{ 2b^3(b-1) \right. \\
& + k(4k-3)b^2\lambda^2 - \left[2b(b-1) + k(2k-1)\lambda^2 \right] m^2 \left. \right\} \\
& + 2kb \left[(4k-3)b^2 + k(k-1)(2k-3)\lambda^2 \right. \\
& \left. - (2k-1)m^2 \right] \tilde{\lambda} + 4k^2(k-1)b(b+1)\tilde{\lambda}^2, \quad (43)
\end{aligned}$$

$$\begin{aligned}
\zeta \equiv & 2(2k-1)b(b-1)(b^2-m^2) \\
& + (12k^2-6k-1)b^3\tilde{\lambda} - (2k-1)(4k+1)bm^2\tilde{\lambda} \\
& + kb(12k^2b-14kb+3b+4k^2-4k)\tilde{\lambda}^2 \\
& - k(2k-1)^2m^2\tilde{\lambda}^2 + 2k^2(k-1)(2k-3)b\tilde{\lambda}^3. \quad (44)
\end{aligned}$$

And $\beta_{n_z n_s m}$ in equation (41) with the variational Gaussian ground-state wave function simplifies to

$$\begin{aligned}
\beta_{n_z n_s m} = & \frac{\left[(b^2+m^2)(2k-1) + 2b\lambda^2 k^2 \right] \left[\tilde{\omega}_{n_z n_s m}^2(\infty) - (b+\lambda^2 k) \right]}{b\lambda^2 k \left[b(4k-3) + 2\lambda^2 k(k-1) \right] + \left[b^3 - (b+\lambda^2 k)m^2 \right] (2k-1)}. \quad (45)
\end{aligned}$$

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