Analytical Method for Yrast Line States in Interacting Bose-Einstein Condensates

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We propose a method to investigate the energy eigenvalue problem and corresponding yrast line for harmonically trapped interacting N-boson systems. This method is particularly simple and effective to obtain the explicit analytical expressions of low-L energy eigenstates with L denoting systems' total angular momentum but with an arbitrarily large N. We have derived the explicit analytical results for $L = 0, 1, \ldots, 9$ and discussed the yrast line for these low-L energy eigenstates.

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Over the last few years, there has been considerable effort focused on the low-lying excitations of atomic Bose-Einstein condensates in harmonic traps [1-7], particularly on the low-lying excitations when condensates have nonzero total angular momentum [3-6]. Mottelson has studied the yrast line of weakly interacting N-boson systems [3], i.e., the ground states at nonvanishing angular momentum L. The case of weakly attractive interaction has been studied by Wilkin et al. [4]. Recently, Bertsch and Papenbrock have numerically investigated the yrast line for harmonically trapped N-boson systems with weak contact interaction [5]. Based on the works of Wilkin et al. [4] and their own numerical computation for N = 25, Bertsch and Papenbrock have made a conjecture on the yrast state expressions for $L \leq N$. However, confirming the conjecture does not appear to be an easy task for large Neven with very small L due to that extremely large Fock space dimension involved when the particle number N is huge. As a matter of fact, no effective method seems to exist yet to obtain either analytically or numerically the energy eigenvalues and eigenstates of interacting N-boson systems with huge particles even when L is small. This immediately leads to another unsolved question whether or not their conjectured states are indeed the yrast states, i.e., the ground states for a given L and for a fixed but huge N. It appears therefore desirable to develop a simple and effective method to investigate the energy eigenvalue problem of interacting N-boson systems in general and the corresponding yrast line in particular.

In this Letter, we shall present such a method which turns the problem of the energy eigenvalue problem of interacting N-boson systems with or without a total angular momentum L into seeking polynomial solutions to a second order linear differential equation. It turns out that this method is particularly simple and effective to obtain the explicit analytical expressions of low-L energy eigenstates and eigenvalues of (either weakly or strongly) interacting N-boson systems with an arbitrary N, and hence fully solve the corresponding yrast line problem for low-L cases. We have given the corresponding explicit analytical results for L = 0, 1, ..., 9 with arbitrarily large N by means of a very simple MATHEMATICA program, and discuss the yrast line for these low-L cases. Let us first consider a fairly universal Hamiltonian containing two-body interactions,

$$H = \sum_{j=0}^{\infty} \omega_j a_j^{\dagger} a_j + \sum_{i,j,k,l=0}^{\infty} \delta_{i+j,k+l} V_{i,j;k,l} a_i^{\dagger} a_j^{\dagger} a_k a_l,$$
(1)

where a_j^{\dagger} and a_j are creation and annihilation operators of the *j*th boson, $V_{i,j;k,l}$ characterizes two-body interactions among bosons, and it can be either weak or strong. N = $\sum_{j=0}^{\infty} n_j$, the eigenvalue of the conserved quantity $\hat{N} =$ $\sum_{i}^{T} a_{i}^{\dagger} a_{j}$, is the total number of bosons. The Kronecker symbol $\delta_{i+j,k+l}$ implies that two-body interactions do not change another conserved quantity $\hat{L} = \sum_{j=0}^{\infty} ja_j^{\dagger}a_j$ with its eigenvalue $L = \sum_{j=0}^{\infty} jn_j$. Several points need clari-fying further here. First, the upper limit ∞ in all the above summation can be replaced by L, for example, L = $\sum_{j=0}^{\infty} jn_j \rightarrow L = \sum_{j=0}^{L} jn_j$, for a fixed *L*. Second, we shall call non-negative *L* as an angular momentum in this paper just as was done in studying trapped Bose-Einstein condensate (BEC) [4,5]. But it should be kept in mind that this name rather easily causes confusion since it at most represents one component of an angular momentum for trapped BEC. In this paper, the name angular momentum merely represents $L = \sum_{j=0}^{\infty} jn_j$. Third, the labeling of bosons throughout the paper begins not from a negative integer but from zero, and hence there exist no quantities such as n_{-1} , a_{-2} , etc. The labeling beginning from a minus integer is obviously equivalent to our labeling way; for instance, a quantity $A = \sum_{n=-J}^{J} B_n$ is equal to $\sum_{n=0}^{2J+1} C_n$ with $C_n = B_{n+J}$.

Our task is to develop a novel method to solve the eigenvalue equation $H|\Psi\rangle = E|\Psi\rangle$. To achieve this goal, we first put the eigenkets $|\Psi\rangle$ into form

$$|\Psi\rangle = F(a_0^{\dagger}, a_1^{\dagger}, \dots, a_j^{\dagger}, \dots, a_L^{\dagger}) |\text{vac}\rangle, \qquad (2)$$

where $|\text{vac}\rangle$ denotes the vacuum state satisfying $a_j|\text{vac}\rangle = 0$ for j = 0, 1, 2, ..., and F is the linear combination of the terms $\prod_j a_j^{\dagger n_j}$ subject to the two constraints $\sum_{j=0}^{\infty} n_j = N$ and $\sum_{j=0}^{\infty} jn_j = L$ for nonnegative integers n_j and L. Here we have made use of

the fact that $\hat{N} = \sum_{j=0}^{\infty} a_j^{\dagger} a_j$ and $\hat{L} = \sum_{j=0}^{\infty} j a_j^{\dagger} a_j$ are two conserved quantities since $[\hat{N}, H] = [\hat{L}, H] = 0$. In other words, $|\Psi\rangle = F|\text{vac}\rangle$ is the common eigenket of H, \hat{N} , and \hat{L} with eigenvalues E, N, and L, respectively. The eigenvalue equation can be rewritten as $EF|\text{vac}\rangle = HF|\text{vac}\rangle = [H, F]|\text{vac}\rangle$ due to $H|\text{vac}\rangle =$ 0. Utilizing $[a_k^{\dagger}a_l^{\dagger}, F] = 0$ (since F contains only creation operators), $[a_m, F] = \partial F/\partial a_m^{\dagger}$, $[a_m a_j, F]|\text{vac}\rangle \equiv$ $[a_m, [a_j, F]]|\text{vac}\rangle$ resulted from $[a_m a_j, F] = [a_m, [a_j, F]] + 2[a_m, F]a_j + (a_m Fa_j - a_j Fa_m), a_j|\text{vac}\rangle = 0$ for j = 0, 1, 2, ..., and $[a_m, [a_j, F]] = \partial^2 F/\partial a_m^{\dagger} \partial a_j^{\dagger}$, it is then straightforward to show from the eigenvalue equation or $EF|\text{vac}\rangle = HF|\text{vac}\rangle = [H, F]|\text{vac}\rangle$ that the polynomial function F satisfies the following differential equation:

$$\sum_{j=0}^{L} \omega_j \xi_j \frac{\partial F}{\partial \xi_j} + \sum_{j,k,l=0}^{L} V_{k+l-j,j;k,l} \xi_{k+l-j} \xi_j \frac{\partial^2 F}{\partial \xi_k \partial \xi_l} = EF,$$
(3)

where $\xi_j \equiv a_j^{\dagger}, j = 0, 1, 2, ..., L$ are L + 1 creation operators, and the polynomial function $F \equiv F(\xi_0, \xi_1, ..., \xi_L)$ is the linear combinations of the terms $\prod_{j=0}^{j=L} \xi_j^{n_j}$ subject to the two constraints $\sum_{j=0}^{L} n_j = N$ and $\sum_{j=0}^{L} jn_j = L$. In the case $\omega_j = j\omega$, Eq. (3) can be further simplified as

$$\sum_{j,k,l=0}^{L} V_{k+l-j,j;k,l} \xi_{k+l-j} \xi_j \frac{\partial^2 F}{\partial \xi_k \partial \xi_l} = (E - \omega L) F,$$
(4)

since the free Hamiltonian $H_0 = \sum \omega_j a_j^{\dagger} a_j$ for $\omega_j = j\omega$ becomes $H_0 = \omega \hat{L}$ so that $\sum_{j=0}^{L} \omega_j \xi_j \frac{\partial F}{\partial \xi_j} = \omega LF$ due to $\hat{L}F = LF$. The problem of obtaining the energy eigenstates and energy eigenvalues has now been turned into finding the polynomial solutions to a second order linear partial differential equation (3) or (4) when $\omega_j = j\omega$.

Let us apply our novel method to study a particular model where $\omega_j = j\omega$ and $V_{ij;kl} = g(k + l)!/(2^{k+l}\sqrt{i!j!k!l!})$. This particular model describes N bosons in a two-dimensional harmonic trap interacting via a contact interaction according to the model utilized by Bertsch and Papenbrock [5]. Regarding discussions of the valid range for contact interaction models, readers are referred to Ref. [7]. It is readily shown that Eq. (4) for $\omega_j = j\omega$ and $V_{ij;kl} = g(k + l)!/(2^{k+l}\sqrt{i!j!k!l!})$ becomes

$$\sum_{M=0}^{L} \sum_{m,k=0}^{M} \frac{M! x_k x_{M-k}}{2^M m! (M-m)!} \frac{\partial^2 F}{\partial x_m \partial x_{M-m}} = \lambda F, \quad (5)$$

where $\lambda = (E - \omega L)/g$ or energy eigenvalue $E = \omega L + g\lambda$, $x_j = \xi_j/\sqrt{j} \equiv a_j^{\dagger}/\sqrt{j}, j = 0, 1, 2, ..., L$ are L + 1 creation operators, and $F \equiv F(x_0, x_1, ..., x_L)$ are the linear combinations of the terms $\prod_{j=0}^{j=L} x_j^{n_j}$ subject to the two constraints $\sum_{j=0}^{L} n_j = N$ and $\sum_{i=0}^{L} jn_i = L$.

We shall use $F[N, L, \lambda]$ to denote the nonzero polynomial solution to Eq. (5), i.e., $F[N, L, \lambda] |vac\rangle = |N, L, \lambda\rangle$ with $|N, L, \lambda\rangle$ describing the common (possibly unnormalized) eigenstate of the three operators $\sum_{i} a_{i}^{\dagger} a_{i}$, $\sum_{i} j a_{i}^{\dagger} a_{i}$, and H with eigenvalues N, L, and $E = \omega L + g\lambda$, respectively. The ket vectors $|N, L, \lambda\rangle$ will be simply called energy eigenstates hereafter. Before solving Eq. (5) to obtain the energy eigenstates and energy eigenvalues of interacting trapped bosons, let us discuss briefly Eq. (3). These discussions are suitable for Eqs. (4) and (5) as well. First, in seeking its polynomial solutions F, we can neglect its operator-type characteristic by regarding its L + 1 operator variables x_k as *c*-number variables due to the fact that all the operators involved in the equation are creation ones and hence mutually commutative. This greatly simplifies the solving procedure. Second, let p(L) denote the multiplicity of the partitions of the non-negative integer L (characterizing total angular momentum) into positive integers, and one then easily sees that the polynomial function F is the linear combination of at most p(L) terms of the form In the combination of a most p(L) terms of the form $\prod_{j=0}^{j=L} x_j^{n_j}$ with $\sum_{j=0}^{L} n_j = N$ and $\sum_{j=0}^{L} jn_j = L$ [for instance, the general form of polynomial function for L = 4 is $F = \alpha x_0^{N-1} x_4 + \beta x_2^2 x_0^{N-2} + \gamma x_1 x_3 x_0^{N-2} + \gamma x_0^{N-3} x_1^2 x_2 + \sigma x_1^4 x_0^{N-4}$ due to p(4) = 5]. In other words, we need only to solve the eigenvalue problem of a $p(L) \times p(L)$ matrix to obtain all the [at most p(L)] energy eigenstates for a fixed L even in a large-N limit. This fact allows us to quickly obtain explicitly the analytical expressions of low-L energy eigenstates and eigenvalues even when the particle number N is very large as will be seen shortly. At this time, it is worthwhile to mention that the *explicit and analytical* results even in the case of very low-L states appear unobtainable by any previous analytical or numerical method even for a rather modest particle number N (say, N = 100 [5]) not to mention for an arbitrarily large N. However, it is a fairly simple matter for us to obtain the explicit results for low-L states but with an arbitrary N. Let us illustrate this point by considering $L = 0, 1, \dots, 9$ but with an arbitrary $N \ge L$ below.

L = 0 case: One and only one polynomial solution in this case is easily seen to be $F[N, L = 0, \lambda = N(N - 1)] = a_0^{\dagger N} / \sqrt{N!}$.

L = 1 case: The unique polynomial solution in this case is also easy to obtain and is given by $F[N, L = 1, \lambda = N(N - 1)] = a_1^{\dagger} (a_0^{\dagger})^{N-1} / \sqrt{(N - 1)!}$.

Using a very simple MATHEMATICA program [8], we have calculated the eigenvalues λ of Eq. (5) (energy eigenvalues $E = \omega L + g\lambda$ but we shall sometimes call λ as energy eigenvalues or eigenvalues for simplicity) for $L = 2, 3, \dots, 9$. Some of the eigenvalues for these L values can be put into the forms

$$\lambda_j^{(L)} = N\left(N - 1 - \frac{j}{2}\right), \qquad j = 0, 2, 3, 4, \dots, L.$$
(6a)

$$\lambda_{L+1}^{(L)} = N^2 - \frac{11}{4}N + \frac{3}{2}, \qquad L \ge 4.$$
 (6b)

$$\lambda_{L+2}^{(L)} = N^2 - \frac{23}{8}N + \frac{3}{2}, \qquad L \ge 5.$$
 (6c)

We conjecture that Eq. (6) also represents eigenvalues for $L \ge 10$ [9]. Note $\lambda_0^{(L)}$ and $\lambda_L^{(L)}$ are, respectively, biggest and smallest eigenvalues among the above listed eigenvalues for a given *L*. For the cases of L = 2, 3, Eq. (6) gives all their eigenvalues [note p(2) = 2 and p(3) = 3]. Equations (6a) and (6b) give all the five [p(4) = 5] eigenvalues for L = 4, while Eqs. (6a), (6b), and (6c) give all the seven [p(5) = 7] eigenvalues for L = 5. Though the eigenvalues can still be calculated by the program [8] when $L \ge 6$, it is found that besides the eigenvalues listed in Eq. (6), there occur some other eigenvalues whose forms are rather complicated (not listed here). In addition, the numbers of the real eigenvalues for these *L* values are all less than

p(L) due to the presence of some complex eigenvalues. These complex eigenvalues do not correspond to reasonable energy eigenvalues and should be discarded. Because of these features, the MATHEMATICA program given in Ref. [8] becomes much less efficient in calculating eigenstates for $L \ge 6$, and we have to develop a new program to overcome the hindrance which will be discussed elsewhere. However, the program takes only minutes to give the analytical expressions of eigenstates for L = 2, 3, 4, 5. We list those for L = 2, 3 below for illustrating purposes.

L = 2 case: The two and only two solutions for $N \ge L$ in this case are

$$F[N, L = 2, \lambda_0^{(2)}] = [(N - 1)a_1^{\dagger 2} + \sqrt{2} a_0^{\dagger} a_2^{\dagger}] (a_0^{\dagger})^{N-2},$$
(7a)

$$F[N, L = 2, \lambda_2^{(2)}] = [a_1^{\dagger 2} - \sqrt{2} a_0^{\dagger} a_2^{\dagger}] (a_0^{\dagger})^{N-2}.$$
 (7b)

L = 3 case: The three and only three solutions for $N \ge L$ in this case are

$$F[N, L = 3, \lambda_0^{(3)}] = \left[2a_0^{\dagger 2}a_3^{\dagger} + 2\sqrt{3}\left(N - 1\right)\left(N - 3\right)a_0^{\dagger}a_1^{\dagger}a_2^{\dagger} - \sqrt{6}\left(N - 1\right)\left(N - 2\right)a_1^{\dagger 3}\right]\left(a_0^{\dagger}\right)^{N-3},$$
(8a)

$$F[N, L = 3, \lambda_2^{(3)}] = \left[\sqrt{6} a_0^{\dagger 2} a_3^{\dagger} + \sqrt{2} (N - 3) a_0^{\dagger} a_1^{\dagger} a_2^{\dagger} - (N - 2) a_1^{\dagger 3}\right] (a_0^{\dagger})^{N-3},$$
(8b)

$$F[N, L = 3, \lambda_3^{(3)}] = [3a_0^{\dagger 2}a_3^{\dagger} - 3\sqrt{3}a_0^{\dagger}a_1^{\dagger}a_2^{\dagger} + +\sqrt{6}a_1^{\dagger 3}](a_0^{\dagger})^{N-3}.$$
(8c)

The eigenstates in Eqs. (7) and (8) can easily be normalized by the method: expressing *F* as the linear combination of the terms of the form $\prod_{j=0}^{L} \eta_{j;n_j}$, $\eta_{j;n_j} = a_j^{\dagger n_j} / \sqrt{n_j!}$ with coefficients α, β, \ldots , then multiplying *F* by $C = 1/\sqrt{|\alpha|^2 + |\beta|^2 + \ldots}$ results in a normalized eigenstate.

In the above, we have illustrated our method by deriving the explicit expressions of energy eigenvalues and eigenstates for low-*L* values with an arbitrary $N \ge L$. We could also easily derive the explicit results for $L \ge N$ so long as *L* or *N* values are not too large. For instance, the explicit results for N = 2 but with an arbitrary positive integer *L* are derived and are given by

$$F[N = 2, L, \lambda = 0] = \sum_{k=0}^{L} (-1)^k \frac{a_k^{\dagger} a_{L-k}^{\dagger}}{\sqrt{k! (L-k)!}}, \quad (9a)$$

$$F[N = 2, L, \lambda = 2] = \sum_{k=0}^{L} \frac{a_k^{\dagger} a_{L-k}^{\dagger}}{\sqrt{k! (L-k)!}}.$$
 (9b)

It is interesting to note that the eigenvalue $g\lambda$ of the two-body interaction operator is zero for the states in Eq. (9a). This property manifests that a two-particle system with two-body interaction can stay in many non-interacting composite states with each of them having different angular momentums, and may carry implication

in the study of the quantum interference and quantum computation (avoiding quantum decoherence, for instance) for the ultracold atoms or ions.

Let us now consider the yrast line for these low-L cases, and prove that they agree with what Bertsch and Papenbrock have conjectured [5]. It can be shown that $\lambda_L^{(L)}(\lambda_0^{(L)})$ for L = 2, 3, ..., 9 are the smallest (biggest) eigenvalues among those listed in Eq. (6) and other real but complicated eigenvalues (for $L \ge 6$) not listed in that equation as well for a fixed L, and therefore the energy eigenstates corresponding to eigenvalues $\lambda_L^{(L)}$ are indeed the ground state or yrast line with the given total angular momentum *L* for the repulsive two-body attraction g > 0, and all these eigenvalues have the form $\lambda_L^{(L)} = N(N - 1 - L/2)$ just as Bertsch and Papenbrock have conjectured. Note that the interaction energy per unit of angular momentum for these ground states has, in units of N|g|, the form (N-1)/L - 1/2, implies that the quadrupole (L=2)mode has the greatest energy gain per unit of angular momentum just as Mottelson pointed out [3]. In addition, the energy per particle $\bar{E} = E/N \equiv \omega(L/N) +$ $g\lambda/N$ in macroscopic limit $N \to \infty$ is readily seen to be $\overline{E} \rightarrow \omega(L/N) + \overline{g}$ for λ given in Eqs. (6b) and (6c), and $\bar{E}_{j} \rightarrow \omega(L/N) + \bar{g}(1 - 0.5jN^{-1}), j = 0, 2, 3, \dots, L$ for λ given in Eq. (6a). Here $\bar{g} = gN$ is a finite quantity in macroscopic limit since the interacting parameter g is inversely proportional to the BEC's volume or the total

particle number N. These results manifest that the energy per particle for all the eigenvalues λ in Eq. (6) is identical to \bar{g} if $L/N \rightarrow 0$ in macroscopic limit. Our next task is to show that all the eigenstates $|N, L, \lambda_s^{(L)}\rangle$ for L = 2, 3, 4, 5are indeed of the forms as Bertsch and Papenbrock conjectured [5]. Here we present the proof for L = 2, 3 (the cases L = 4, 5 can be shown by following the same proof procedure). To reach this goal, we first briefly review some of the basic facts. The normalized single-particle state is of the form $z^k \exp(-|z|^2/2)/\sqrt{\pi k!} \equiv (z^k/\sqrt{k!})\Psi_{\text{vac}}$ where z = x + iy describe the single-particle position in the two-dimensional harmonic trap [4]. For an N-particle system, the creation operator a_k^{\dagger} creates, from the vacuum state, a symmetric state $\propto (\sqrt{k})^{-1} \sum_{j=1}^{N} z_j^k |\text{vac}\rangle$. We have the following corresponding relation:

$$\sum_{k=1}^{N} z_{k}^{j} \longleftrightarrow \sqrt{j!} a_{j}^{\dagger} \frac{(a_{0}^{\dagger})^{N-1}}{(N-1)!}, \qquad j = 2, 3, \dots \quad (10a)$$

$$\sum_{i_1 > \dots > i_n} z_{i_1} z_{i_2} \cdots z_{i_n} \iff \frac{m_1}{n!} \frac{(n_0)}{(N-n)}, \qquad 2 \le n \le N.$$
(10b)

$$\sum_{\substack{i \neq j_1, \dots, i \neq j_k}}^{j_1 > \dots > j_k} z_i^m z_{j_1} \cdots z_{j_k} \iff \sqrt{m!} a_m^{\dagger} \frac{a_1^{\dagger k}}{k!} \frac{(a_0^{\dagger})^{N-1-k}}{(N-1-k)!},$$
$$m = 2, 3, \dots, N; \qquad k = 1, 2, \dots, N-1.$$
(10c)

The summations in Eq. (9) are all from 1 to N subject to the confinements designated explicitly. Let $z_c = \sum_{i=1,N} z_i/N$ be the center of mass, note $(z_i - z_c) = \sum_{j=1}^{N} (\delta_{ij} - 1/N) z_j$, and we can show

$$\sum_{i>j} (z_i - z_c) (z_j - z_c) = -\frac{(N-1)}{2N} \sum_{k=1}^N z_k^2 + \frac{1}{N} \sum_{i>j} z_i z_j,$$
(11a)

$$\sum_{i>j>k} (z_i - z_c) (z_j - z_c) (z_k - z_c) = \frac{(N-1)(N-2)}{3N^2} \sum_{k=1}^N z_k^3 - \frac{(N-2)}{N^2} \sum_{i\neq j} z_i^2 z_j + \frac{4}{N^2} \sum_{i>j>k} z_i z_j z_k.$$
 (11b)

It is then straightforward to prove $|N, L, \lambda_L^{(L)}\rangle \sim \sum_{i_1 > i_2 > \cdots > i_L} (z_{i_1} - z_c) (z_{i_2} - z_c) \cdots (z_{i_L} - z_c) |vac\rangle$ for L = 2, 3, 4, 5 (we have omitted the proof for L = 4, 5 here due to page limit), just as the forms conjectured by Bertsch and Papenbrock [5].

In summary, we have developed a novel method by which the energy eigenvalue problem for fairly universal systems with (either weak or strong) two-body interactions is turned into solving a second order linear partial differential equation. It appears that there exists no systematical and effective method yet to deal with such systems, especially when there exist sufficiently large modes to involve in strong two-body interactions. Applying this method to study the energy eigenvalue problem and corresponding yrast line for harmonically trapped interacting N-boson systems via a particular model, we have found that it is particularly simple and effective to obtain the explicit analytical expressions of low-L energy eigenstates with arbitrarily large N. Another advantage of our method is that it can directly express analytically energy eigenstates in Fock space so as to avoid using somewhat complicated Schrödinger representation.

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