Calculation of atomic number states: a Bethe ansatz approach

Shou-Pu Wan\textsuperscript{1,2,3}, Mark G Raizen\textsuperscript{1,2} and Qian Niu\textsuperscript{1}

\textsuperscript{1} Department of Physics, The University of Texas, Austin, TX 78712, USA
\textsuperscript{2} Center for Nonlinear Dynamics, The University of Texas at Austin, TX 78712, USA
E-mail: swan@physics.utexas.edu

Received 24 July 2009, in final form 11 August 2009
Published 22 September 2009
Online at stacks.iop.org/JPhysB/42/195506

Abstract
We analyse the conditions for producing atomic number states in a one-dimensional optical box using the Bethe ansatz method. This approach provides a general framework, enabling the study of number state production over a wide range of realistic experimental parameters.

1. Introduction

The realization of Bose–Einstein condensation (BEC) in dilute gases has enabled the study and control of many-body systems. While most of the work has focused on the properties and excitations of the condensate, it has provided a new path towards generation of atomic number (or Fock) states. These few body states with a definite number of atoms in the ground state are of great interest for quantum information where individual qubits can be addressed \cite{1–3}, and could also be important for atom interferometry in order to reach the Heisenberg limit of detection. Experimentally, realization of Fock states requires a BEC confined in an optical box coupled with single-atom counting. The challenge is to obtain confinement in a trap that is comparable to optical lattices, but with only a single site \cite{4}. Recent experimental work has demonstrated all the necessary steps towards this goal and they are now being incorporated into a single system \cite{5}. In parallel, the theoretical analysis of this problem has focused on the conditions for optimum number state production \cite{6, 7}. These include the role of varying trap depth and size, either separately or in tandem. The interaction strength is a third control parameter that can be tuned with the help of Feshbach resonances or by tuning the transverse confinement of the optical trap \cite{4, 8} and is considered here in more detail.

It is clear that strong repulsion between atoms are desirable for the production of number states. The infinitely strong interaction regime is the so-called Tonks–Girardeau regime where calculation has been made trivial thanks to the boson–fermion correspondence \cite{9}. However, this is only an unreachable limiting case. To make realistic predictions about what can be experimentally realized, we must consider the regime of relatively but not infinitely strong interactions. Previous studies of this regime were carried out using direct diagonalization which is both time consuming and lacks scalability in the interaction strength. In this paper, we develop an approach that takes interaction as a parameter and by which we are able to chart number states in the parameter space with interaction as one of its dimensions\textsuperscript{4}.

Our calculation of atomic number states in a 1D optical box is based on the so-called Bethe ansatz approach. This method was first developed by Hans Bethe to solve the problem of a one-dimensional (1D) spin-1/2 Heisenberg ferromagnet \cite{10}. Since its invention, Bethe’s method has found important applications in the study of interacting spin systems \cite{11–13}. It has also been applied to solve the problem of a 1D bosonic gas with repulsive $\delta$-function interactions \cite{14–20}. An outline for the structure of this paper is as follows. In section 2, we formulate the problem; in section 3, we present approximate solutions to our problem with the Bethe ansatz approach; in section 4, we use Bethe ansatz solutions to analyse issues related to number state production.

2. Formulation of the problem

The problem of many bosons with a $\delta$-function interaction trapped in 1D square well potential with finite well depth was

\textsuperscript{4} There are other technical reasons in tuning the interaction strength. To facilitate efficient loading of Bose–Einstein condensate into the optical box, the transverse trapping frequency is often relaxed in the beginning and tightened up towards the end to promote atom–atom interaction. This process often gets involved with that of the number state production. Therefore, we need to study the connections across various interaction regimes.
studied using the Bethe ansatz in [20]. We find that the problem of producing Fock states in the ultracold atom systems trapped in 1D optical box bears similar characteristics. We treat the 1D optical trap as a square well potential of length $L$ and depth $V_0$. We write the interaction potential as $\frac{4a}{a_\perp^2}c\delta(x_i - x_j)$, where $x_i$ and $x_j$ are the positions of the interacting particles, $h$ is Planck’s constant and $m$ is an atom’s mass, and $c$ is the interaction strength and has dimension of $[1/\text{length}]$. According to [21] we have the following expression for $c$:

$$
  c = \frac{4a}{a_\perp^2} \left( 1 - \frac{C}{a} \right)^{-1},
$$

where $a$ is the s-wave scattering length in a three-dimensional space, $a_\perp = \sqrt{\frac{2\hbar^2}{m\omega_\perp}}$, $\omega_\perp$ is the transverse trapping frequency and $C \approx 1.4603$ is an empirical constant number. Since the interaction strength $c$ depends on both scattering length and transverse trapping frequency $\omega_\perp$, tuning either of them will affect the interaction strength. The transverse trapping frequency may be controlled by optical box parameters [4]. Scattering length may be adjusted by Feshbach resonance [8]. To give a sense of order of magnitude, we denote the wavefunctions in a region of $x$, the total energy of the Bethe ansatz state is $E = -\sum_j k_j^2/2 = \sum_j (k_j^2 - k_0^2)/2$. The eigenfunction (wavefunction) of equation (4) is piecewise continuous in the $N$-dimensional coordinate space $\{x_1, x_2, \ldots, x_N\}$. For simplicity, we consider three representative regions in the $N$-dimensional coordinate space:

$$
  R_1 = -x_0/2 < x_1 < x_2 < \cdots < x_N < x_0/2, \\
  R_2 = x_1 < -x_0/2 < x_2 < \cdots < x_N < x_0/2, \\
  R_3 = -x_0/2 < x_1 < \cdots < x_{N-1} < x_0/2 < x_N.
$$

$R_1$ represents a region where all particles are trapped; $R_{2,3}$ represent a region where the first (third) particle tunnels into the left (right) barrier. In fact, each of these regions falls in a class consisting of $N!$ regions that are related by coordinate permutation. For ease of reference, we name $A$ the class of regions that can be obtained from $R_1$ by mere coordinate permutations and study the wavefunctions in these regions at once.

We denote the wavefunctions in a region of $A$ as $\phi_\tau(A)$, where $\tau$ is the permutation operator that transforms $R_1$ into this region, i.e. $R_\tau = \tau R_1$. This wavefunction is the superposition of pure plane waves with ‘$\pm$ signs’ times permuted wave numbers,

$$
  \phi_\tau(A) = \sum_{\zeta \in C_N^2} \sum_{\sigma \in G} A(\zeta, \sigma; \tau) e^{i(\sigma A - \zeta)},
$$

where $\zeta = \{\zeta_1, \zeta_2, \ldots, \zeta_N\}$ represents a possible combination of $N$ signs each of which is either $+$ or $-$ and $C_N^2$ represents the group of such operations, $G$ is the permutation group of $N$ particles and $A(\zeta, \sigma; \tau)$ is the superposition amplitude.

It is clear that the superposition amplitude $A(\zeta, \sigma; \tau)$ is a functional of the sign-flipping operator, the wave number permutation operator and the region permutation operator. By bosonic particle permutation symmetry, we establish the first set of equations among the superposition amplitudes,

$$
  A(\zeta, \sigma; \tau) = A(\zeta, \tau; \sigma; I),
$$

where $I$ is the identity element in the permutation group.

The wavefunctions in region $R_2$ have a more complicated form,

$$
  \phi_2(A) = \sum_{\zeta} \sum_{\sigma \in G} B(\zeta, \sigma) e^{i(\sigma A - \zeta)} \phi_{\zeta} \sum_{j=1}^N (\zeta \sigma A - A)_{j},
$$

where $(\zeta \sigma A - A)_{j}$ is the $j$th component wave number after the permutation operation $\sigma$ and the sign-flipping operation $\zeta$. $(\zeta \sigma A - A)_{j}$, which can be regarded as an extra operator on top of the permutation operation $\sigma$, and $B(\zeta, \sigma)$ is the superposition amplitude. Similarly, the wavefunctions in region $R_3$ may be written as

$$
  \phi_3(A) = \sum_{\zeta} \sum_{\sigma \in G} C(\zeta, \sigma) e^{i(\sigma A - \zeta)} \phi_{\zeta} (\sigma A)_{x_N}.
$$

3. Bethe ansatz solutions

In section 2, we defined a boundary value problem for the interacting many-atom system. In this section, we will obtain solutions using the Bethe ansatz.

As studied in previous literatures [14, 16, 20], Bethe ansatz solution of this problem introduces a set of $N$ as-yet-unknown wave numbers $\vec{k} = \{k_1, k_2, \ldots, k_N\}$. In conjugate to these wave numbers, another set $\vec{k}' = \{k_1', k_2', \ldots, k_N'\}$ is defined as

$$
  k_j' = \sqrt{k_j^2 - k_0^2},
$$

for $j = 1, 2, \ldots, N$. The total energy of the Bethe ansatz state is $E = -\sum_j k_j^2/2 = \sum_j (k_j'^2 - k_0^2)/2$. The eigenfunction (wavefunction) of equation (4) is piecewise continuous in the $N$-dimensional coordinate space $\{x_1, x_2, \ldots, x_N\}$. For simplicity, we consider three representative regions in the $N$-dimensional coordinate space:

$$
  R_1 = -x_0/2 < x_1 < x_2 < \cdots < x_N < x_0/2, \\
  R_2 = x_1 < -x_0/2 < x_2 < \cdots < x_N < x_0/2, \\
  R_3 = -x_0/2 < x_1 < \cdots < x_{N-1} < x_0/2 < x_N.
$$

$R_1$ represents a region where all particles are trapped; $R_{2,3}$ represent a region where the first (third) particle tunnels into the left (right) barrier. In fact, each of these regions falls in a class consisting of $N!$ regions that are related by coordinate permutation. For ease of reference, we name $A$ the class of regions that can be obtained from $R_1$ by mere coordinate permutations and study the wavefunctions in these regions at once.

We denote the wavefunctions in a region of $A$ as $\phi_\tau(A)$, where $\tau$ is the permutation operator that transforms $R_1$ into this region, i.e. $R_\tau = \tau R_1$. This wavefunction is the superposition of pure plane waves with ‘$\pm$ signs’ times permuted wave numbers,

$$
  \phi_\tau(A) = \sum_{\zeta \in C_N^2} \sum_{\sigma \in G} A(\zeta, \sigma; \tau) e^{i(\sigma A - \zeta)},
$$

where $\zeta = \{\zeta_1, \zeta_2, \ldots, \zeta_N\}$ represents a possible combination of $N$ signs each of which is either $+$ or $-$ and $C_N^2$ represents the group of such operations, $G$ is the permutation group of $N$ particles and $A(\zeta, \sigma; \tau)$ is the superposition amplitude.

It is clear that the superposition amplitude $A(\zeta, \sigma; \tau)$ is a functional of the sign-flipping operator, the wave number permutation operator and the region permutation operator. By bosonic particle permutation symmetry, we establish the first set of equations among the superposition amplitudes,

$$
  A(\zeta, \sigma; \tau) = A(\zeta, \tau; \sigma; I),
$$

where $I$ is the identity element in the permutation group.

The wavefunctions in region $R_2$ have a more complicated form,

$$
  \phi_2(A) = \sum_{\zeta} \sum_{\sigma \in G} B(\zeta, \sigma) e^{i(\sigma A - \zeta)} \phi_{\zeta} \sum_{j=1}^N (\zeta \sigma A - A)_{j},
$$

where $(\zeta \sigma A - A)_{j}$ is the $j$th component wave number after the permutation operation $\sigma$ and the sign-flipping operation $\zeta$. $(\zeta \sigma A - A)_{j}$, which can be regarded as an extra operator on top of the permutation operation $\sigma$, and $B(\zeta, \sigma)$ is the superposition amplitude. Similarly, the wavefunctions in region $R_3$ may be written as

$$
  \phi_3(A) = \sum_{\zeta} \sum_{\sigma \in G} C(\zeta, \sigma) e^{i(\sigma A - \zeta)} \phi_{\zeta} (\sigma A)_{x_N}.
$$
where \((\sigma^2)^{N}_{\nu} \equiv \sqrt{k_i^2 - (\sigma^2)^{N}_{\mu} - 2}\) and \(C(\zeta, \sigma)\) is the superposition amplitude.

From equation (5), it is clear that if, for any \(i, k_i > k_0\) then there will be a corresponding pure imaginary \(\kappa_i\). From equations (11) and (12), any pure imaginary \(\kappa_i\) will cause the Bethe ansatz wavefunction unnormalizable. Then from the normalizability requirement stated at the end of section 1, we reason that a Bethe ansatz state is bound if and only if all of the wave numbers are real and smaller than \(k_0\). Since we are primarily interested in bound states, from now on we implicitly mean bound state when we say Bethe ansatz state, unless otherwise stated.

Once we get the Bethe ansatz wavefunctions written down, the rest is straightforward. The main features of equation (4) are the singular \(\delta\)-function particle–particle interaction and the nonzero potential step at the edge of the square well. The Bethe ansatz method elegantly treats both as boundary conditions. The boundary conditions at \(x_i = x_j\) are the solution to the transcendental equation

\[
\frac{\partial \psi}{\partial x_i} \bigg|_{x_i = x_j} = \frac{\partial \psi}{\partial x_j} \bigg|_{x_i = x_j}
\]

and certain discontinuity in their first derivatives on the other,

\[
\left[ \frac{\partial \psi}{\partial x_i} - \frac{\partial \psi}{\partial x_j} \right]_{x_i = x_j} = \left[ \frac{\partial \psi}{\partial x_i} - \frac{\partial \psi}{\partial x_j} \right]_{x_i = x_j}
\]

(14)

The boundary conditions at \(x_i = \pm x_0/2, i = 1, 2, \ldots, N\), require continuity of both wavefunctions and their first derivatives:

\[
\left. \psi \right|_{x_i = x_0/2} = \left. \psi \right|_{x_i = x_0/2} = \left. \frac{\partial \psi}{\partial x_i} \right|_{x_i = x_0/2}
\]

(15)

(16)

Plugging equations (9), (11) and (12) into equations (13), (14), (15) and (16) and including equation (10), we obtain the complete group of equations for our original problem.

For the purpose of this paper, it suffices to keep just the wave numbers and eliminate all other unknowns. Doing so yields the following secular equations for the \(N\) wave numbers,

\[
\pi I_j - x_0 k_j = 2 \sin^{-1} \frac{k_j}{k_0}
\]

\[+ \sum_{j=1}^{N} \left( \tan^{-1} (k_j + k_i) + \tan^{-1} (k_i - k_j) \right), \quad (17)\]

where \(j = 1, 2, \ldots, N\), and \(I = \{I_1, I_2, \ldots, I_N\}\) is a set of preselected integers.

Now a retrospect on the three regions we selected in the coordinate space might make you wonder why we have not included more regions (and more equations), possibly with two or more particles lying outside the trap area simultaneously. In reality, this is possible, but only with small probability for deeply bound state. The effect on the number-state condition should be ignorable. Firstly, insofar as representative limiting cases (strong interaction limit and deep trap limit), Bethe ansatz solution agrees with known results (see figure 2(a)). Secondly, the energy spacings between single-particle levels are big near the strong interaction regime where number state experiments take place most likely and therefore the probability for more than one particle to tunnel into the barrier is ignorably small at all times. For this reason, we argue that the Bethe ansatz-based approach is a sufficiently good approximation to our problem.

There are a few notable aspects of equation (17). Firstly, it is a transcendental equation and so does not have analytic solution. Secondly, we must pick a set of integers \(I = \{I_1, I_2, \ldots, I_N\}\) before we start the numerical computation. Apparently, not any set of integers would lead to a physically meaningful solution. Then a natural question to ask is what does. As argued in appendix A, we find that equation (17) yields valid solution if and only if the set of integers \(I\) are mutually distinct, somewhat similar to the theorem in [16]. A corollary of is that wave numbers thus obtained have mutually distinct absolute values. Because of this one-to-one correspondence, we use the set \(I\) as the quantum numbers for the corresponding Bethe ansatz state.

Besides knowing what set of integers are valid quantum numbers, we need to further identify the ground state and the first excited state. As argued in appendix B, we find that the ground state of an \(N\)-boson system has the quantum number \(\{1, 2, \ldots, N\}\); the first excited state has the quantum number \(\{1, 2, \ldots, N−1, N+1\}\) (see figure 1).

Without loss of generality, we reorganize the set of wave numbers such that \(0 < k_1 < k_2 < \cdots < k_N < k_0\). We define the \(j\)th single particle energy as \(e_j = −k_j^2/2\), for \(j = 1, 2, \ldots, N\). Figure 1 gives total energies of the low-lying Bethe ansatz states.

4. Number states

We now apply the results of the previous sections to the problem of number state production. We can safely assume no
atom with positive energy presents in space near the trapped area. In reality, if an atom acquires positive energy, it would be quickly swept out of the vacuum chamber. Therefore, it is safe to assume that the states in the continuum spectrum are virtually unoccupied all the time.

As dictated by Bethe ansatz, for some given trap parameters (depth $V_0$, trap size $L$, scattering length $a$ and transverse trapping frequency $\omega_\perp$), $N$ bosons can be contained in the trap if and only if there is an $N$-boson Bethe ansatz state. The energy levels for an $N$-boson system have been computed by equation (17) numerically. As an example, figure 2 shows a four-boson Bethe ansatz state that ceases to exist in certain regions of the parameter space. The Bethe ansatz state can only exist down to a certain trap depth in panel (a) and can only exist up to certain interaction strength in panel (b), provided that all other parameters are held unchanged. We call the maximum number of particles that can be contained in the trap the trap capacity. The trap capacity puts an upper bound on the number states for a given point in the parameter space. The whole parameter space is thus partitioned into zones of certain trap capacities. We define the boundaries of these partitions as the ionization threshold, because as we cross the boundaries from higher trap capacity side to lower capacity side adiabatically, the system state changes from stable to unstable and must release some particle(s). In figure 3 we show the ionization threshold for a system of 2, 3, 4, 5 and 6 bosons.

Now that we have a clear upper limit, the trap capacity, on the number state that may be present for a given trap and other physical parameters. It remains questionable whether or not the trap capacity can be reached. The adiabatic laser cooling technique developed in [6] and the simulations in the Tonks–Girardeau region made in [7] seem to suggest that it is possible to reach the trap capacity with the ultracold technique developed in [4, 5].

The starting point is a almost pure Bose–Einstein condensate (BEC) that is optically trapped. Ignore excitation effects for now, it is useful to view the process from the angle of quantum optics and regard the state of the BEC as a coherent state [22]. A coherent state is essentially a superposition of Fock states with a Poisson distribution in the boson numbers. As we adiabatically change experimental parameters from partitions with higher trap capacity to lower capacity targeting some number state, the Bethe ansatz solution puts a tighter restriction on the maximum number state. The system state thus undergoes two changes side by side: (1) more and more high-energy atoms are forced out; (2) more and more high-number Fock states are quantum mechanically ‘projected’ out of the system state (resulting in the so-called

![Figure 2](image-url) - Single particle energies of four sodium atoms in Bethe ansatz ground states. Trap size $L = 5 \, \mu m$. (a) Dependence on interaction strengths $c$. Trap depth $V_0 = k_B \times 25 \, nK$, where $k_B$ is Boltzmann’s constant. The dot-dashed vertical line denotes the maximum interaction strength above which no Bethe ansatz state of four-boson system exists. The other two vertical lines denote the interaction strengths of sodium (dotted) and $^{87}$Rb (dashed) atoms at $\omega_\perp = 2\pi \times 150\, kHz$ and zero magnetic field. Inset: the trap depth is lifted to $k_B \times 40\, nK$, at which condition all four atoms remain trapped to the Tonks limit. (b) Dependence on trap depths ($V_0$). Transverse trapping frequency $\omega_\perp = 2\pi \times 150\, kHz$. Magnetic field is zero. The vertical line (dot-dashed) denotes the minimum trap depth below which no bound state of four-boson system exists. (Colour online.)

![Figure 3](image-url) - Ionization thresholds of sodium atoms with all parameters fixed except trap depth (we use $h^2/L^2$ as energy unit for convenience). Only highest single particle energies of the Bethe ansatz $N$-boson states are shown with $N = 2$ (circles), 3 (squares), 4 (diamond), 5 (upright triangles) and 6 (inverted triangles). Trap size $L = 5 \, \mu m$; transverse trapping frequency $\omega_\perp = 2\pi \times 150\, kHz$. The ionization thresholds (with the current numeric calculation step size) are marked with vertical lines (dot-dashed). (Colour online.)
Under optimal experimental conditions, the process continues until at some point, while the average number $\langle N \rangle > 0$, the number uncertainty $\sigma \approx 0$. A rigorous simulation of this would require calculating the value $\sigma/N$ as a function of time in a dynamic process and is certainly beyond the scope of this paper. In figure 4, we show trap capacities and ionization thresholds as functions of trap depth and size. The interaction strength is implicit in the unit we adopted.

There are several ways to tune the physical parameters to achieve the above goals. In previous references [6, 7], only culling (changing trap depth), squeezing (changing trap size), or some combinations of the two are discussed. In certain circumstances, we propose that atom–atom interaction strength $c$ be possibly tuned to supplement the production of number states. In view of the intrinsic limitations in tuning the trap parameters, it is possible that tuning of interaction strengths could play a key role in number state experiments.

The path to a number state becomes clear now. By tuning the physical parameters of the 1D optical trap adiabatically, we force the ultracold atom sample through a series of quantum collapses until it eventually reaches the desired Fock state with some acceptable fidelity. Ideally, the course connecting the starting point and a targeted Fock state consists of a series of states (the Bethe ansatz states) with well-defined particle number. But in reality, there are always some elementary excitations, which is defined as any deviation from the ideal adiabatic course. Possible elementary excitations include occupations of excited Bethe ansatz state (of the same particle number), earlier ionizations (loss of particles before reaching the Bethe ansatz ionization threshold) and simultaneous ionizations of more than one particle.

We now analyse the effects of excitations. Abrupt changes in the trapping potential tend to introduce extra terms into the system density matrix. As the system gets near an ionization threshold, the system becomes particularly delicate, since the particle with the highest energy can tunnel further away from the centre of the trap and thus external disturbance has bigger exciting effect on the system. Moreover, immediately after the ionization threshold is passed, the system density

---

**Figure 4.** Map of number states and the ionization thresholds for sodium atoms in 1D optical trap in adiabatic limit. Transverse trapping frequency $\omega_\perp = 2\pi \times 150$ kHz and zero magnetic field are assumed. Note that $c^{-1}$ and $\hbar^2 c^2/m$ are used to make the axes dimensionless. (a) Contour plot of number states as function of trap depth and size; (b) and (c) cross-sectional cut views at the indicated trap size ($5 \mu$m) and depth (4 nK) (solid lines) of (a). The ticks on horizontal axes give the calculated ionization thresholds.

**Figure 5.** Excitation energy gaps between ground and first excited states as function of trap depth for two (circles), three (squares), four (diamonds), five (upright triangles) and six (inverted triangles) sodium atoms. Trap size is $5 \mu$m. (Colour online.)
matrix is subject to various excitations due to wavefunction collapses. These excitations are crucial to the fidelity of Fock state production, since they cause significant reversion in the number uncertainty of the final state. A characteristic measurement of tendency of excitation is the energy gap, $\Delta$, which is defined as the difference between total energies of ground and first excited Bethe ansatz states (if both exist). According to our calculation, they are on the order of a few $k_B \times 10$ nK (see figure 5). $\Delta$ puts restrictions in twofold. Firstly, the temperature must be maintained lower than a few 10 nK, otherwise, fidelity could be endangered due to thermal excitation. Furthermore, the energy gap puts a requirement on the adiabaticity condition [23]: the culling speed must be much smaller than $\Delta^2/\sqrt{\hbar}$ to maintain a relatively high fidelity. To give a sense of number, we consider the culling of trapping potential from the ionization threshold of three particles down to that of two particles at trap size of 5 $\mu$m and transverse trapping frequency $\omega_\perp = 2\pi \times 150$ kHz. According to our calculation, the minimum time required to complete this portion of the culling should be no less than 0.3 ms to be considered as adiabatic.

5. Conclusion

In conclusion, we have calculated the conditions for number states of ultracold atoms in an 1D optical trap with the Bethe ansatz approach. This approach provides a new view for the many-body system through the effective single particle levels, and allows efficient calculation of the ionization energies. We have charted ionization thresholds for our many-boson system in the comprehensive parameter space including the interaction strength. We have also discussed the quantum mechanical processes in producing number states in the adiabatic limit and estimated the adiabatic condition by calculating the spectra of excitations.

Acknowledgments

We acknowledge support from the NSF and from the R A Welch Foundation. QN also thanks DoE for support. MGR acknowledges support from Sid W Richardson Foundation. We thank Greg Fiete for inspiring suggestions. SPW would like to thank Tongcang Li, Hrishikesh Kelkar, Shengyuan Yang for the useful discussions.

Appendix A. Valid Bethe ansatz solutions

First of all, we need a change of unit to make the dependence of secular equation on interaction strength explicit. (See section 1 for the previous choice of unit.) To that end, we choose the trap length $L$ as the length unit, $\hbar^2/ mL^2$ as the energy unit. Then the secular equation (17) is transformed to

$$\pi I_j - k_j = 2 \sin^{-1} \frac{k_j}{k_0} + \sum_{l=1}^{N} \left[ \tan^{-1} \frac{k_j + k_l}{c} + \tan^{-1} \frac{k_j - k_l}{c} \right].$$

(A.1)

The secular equations (A.1) depend on the interaction strength, the trap depth and a set of integers. Clearly, the interaction strength and trap depth can assume any positive real values. Next, we study what sets of integers can be used in the secular equations (A.1) to obtain physically meaningful solutions.

Let us take a four-particle system, for example. We assume $k_0 = 10$ for the trap. For the mere purpose of obtaining a solution, we plug $[0, 1, 2, 3]$ into the secular equations (A.1) for an arbitrary interaction strength $c$. As we insert more and more points in the range $[0, c]$, we expect to see the solutions form continuous paths connecting solutions at some finite interaction strengths to that of $c = 0$. The solutions for the case of $c = 0$ can be easily obtained with other methods. Thus we can simply compare that to our solution path—if they do not match, the solutions on the whole path are invalid. Indeed, they are invalid. As one can verify, the integer sets $\{1, 2, 3, 4\}$ and $\{1, 2, 3, 5\}$ are valid, while $\{0, 1, 2, 3\}$ and $\{1, 2, 3, 3\}$ are invalid.

This method can be generalized to any many-particle system with any trap depths and interaction strengths. Our non-exhaustive experiments unanimously show that a Bethe ansatz solution is connected to a solution at $c = 0$ if and only if the set $I$ consists of positive and mutually distinct integers. We also find that for $c \neq 0$, the wave numbers in the solution are mutually distinct if and only if the integers in the set $I$ are mutually distinct.

Appendix B. Order of Bethe ansatz states

With the verification process explained in appendix A, we know that only positive, mutually distinct integers can be supplied to equation (A.1). However, it is still left to determine which integer set gives the ground state, which gives the first excited state, and so on.

In this section, we use a similar method to that used in the previous section to partially order the levels. This time, our clue comes from the solutions in the strong interaction limit $c \rightarrow \infty$. In that case, the ground state of the many-boson system is similar to that of a degenerate-fermion gas because of the boson–fermion correspondence principle [9]. Our numerical calculations show that with the set $I = \{1, 2, \ldots, N\}$, the solution of equation (A.1) approaches that of the ground state of the degenerate fermion system in the limit $c \rightarrow \infty$. We therefore expect that for finite $c$, the ground state is also obtained with this same set. Knowing that $I = \{1, 2, \ldots, N\}$ generates the ground state, it is almost intuitive to see that $I = \{1, 2, \ldots, N-1, N+1\}$ will generate the first excited state. Indeed, experiments with this set of integers for all interaction strengths support this viewpoint.

To summarize, we conclude that for any given $N$, the set $I = \{1, 2, \ldots, N\}$ leads to the ground state and the set $I = \{1, 2, \ldots, N-1, N+1\}$ to the first excited state. However, a general rule for ordering all the energy levels at arbitrary interaction strength is neither simple nor necessary.
References

[1] Jaksch D, Briegel H-J, Cirac J I, Gardiner C W and Zoller P 1999 Phys. Rev. Lett. 82 1975
[2] Dudarev A M, Diener R B, Wu B, Raizen M G and Niu Q 2003 Phys. Rev. Lett. 91 010402
[3] Andersson E and Barnett S M 2000 Phys. Rev. A 62 052311
[4] Meyrath T P et al 2005 Phys. Rev. A 71 041604
Meyrath T P et al 2005 Opt. Express 13 2843
[5] Chuu C-S, Schreck F, Meyrath T P, Hanssen J L, Price G N and Raizen M G 2005 Phys. Rev. Lett. 95 206403
[6] Dudarev A M, Raizen M G and Niu Q 2007 Phys. Rev. Lett. 98 063001
[7] Campo A del and Muga J G 2008 Phys. Rev. A 78 023412
Pons M, Campo A del, Muga J G and Raizen M G 2009 Phys. Rev. A 79 033629
[8] Inouye S et al 1998 Nature 392 151
Courteille Ph, Freeland R S, Heinzen D J, van Abeelen F A and Verhaar B J 1998 Phys. Rev. Lett. 81 69
[9] Girardeau M 1960 J. Math. Phys. 1 516
[10] Bethe H A 1931 Zeitschrift für Phys. 71 205
See also Bethe H A 1997 Selected Works of Hans A. Bethe: With Commentary (Singapore: World Scientific)
(Engl. transl.)
[11] Orbach R 1958 Phys. Rev. 112 309
[12] Walker L R 1959 Phys. Rev. 116 1089
[13] Lieb E, Schultz T and Mattis D 1961 Ann. Phys., NY 16 407
[14] Lieb E H and Liniger W 1963 Phys. Rev. 130 1605
Lieb E H 1963 Phys. Rev. 130 1616
[15] McGuire J B 1964 J. Math. Phys. 5 622
[16] Yang C N 1967 Phys. Rev. Lett. 19 1312
[17] Sutherland B 1968 Phys. Rev. Lett. 20 98
Sutherland B 1980 J. Math. Phys. 21 1770
[18] Hao Y, Zhang Y, Liang J Q and Chen S 2006 Phys. Rev. A 063617
[19] Gaudin M 1967 Phys. Rev. A 24 55
[20] Li Y Q 1995 Phys. Rev. A 52 65
[21] Olshanii M 1998 Phys. Rev. Lett. 81 938
[22] Andrews M R, Townsend C G, Miesner H-J, Durfee D S, Kurn D M and Ketterle W 1997 Science 275 637
[23] Aharonov Y and Anandan J 1987 Phys. Rev. Lett. 58 1593