The Bose molecule in one dimension

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Abstract

We give the Green function, momentum distribution, two-particle correlation function, and structure factor for the bound state of $N$ indistinguishable bosons with an attractive delta-function interaction in one dimension, and an argument showing that this boson “molecule” has no excited states other than dissociation into separated pieces.
I. THE BOSON MOLECULE

Consider a system of \(N\) identical bosons in one dimension, with an attractive delta-function interaction. There is a bound state for all \(N\), having the form of a well-localized "molecule" \([1-3]\). This result is interesting, since it is the unique example of an exactly solved localized many-body system. A possible experimental realization of this system would be in a \(^7\text{Li}\) vapor \([4]\) confined to an atomic trap which is so tight in two directions, that the system can be regarded as one-dimensional with respect to the third direction. Such traps are realistic prospects in the near future \([5]\), and high-aspect ratio cigar-shaped traps approximating quasi-one-dimensional systems are already available experimentally \([6]\).

We seek the localized eigenfunctions \(\Psi\{x_i\}\) of the Hamiltonian

\[
H = - \sum_{i=1}^{N} \frac{\hbar^2}{2m} \frac{d^2}{dx_i^2} - W \sum_{i<j} \delta(x_i - x_j) \tag{1}
\]

wherein \(m\) is the particle mass and \(W\) is a positive parameter representing the strength of interparticle attraction.

The wavefunction and many derived quantities can be given exactly and in closed form; however, it is useful to first consider the mean-field version of this theory. The Gross-Pitaevskii (GP) approximation \([7]\) assumes that \(\Psi\{x_i\}\) can be written as a simple product

\[
\Psi(\{x_i\}) = \prod_i \psi(x_i) \tag{2}
\]

where the \(\psi(x)\) are eigenfunctions for a single particle moving in the average potential of all the others

\[
\epsilon \psi(x) = - \frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x). \tag{3}
\]

where \(V(x) = -(N-1)W|\psi_0(x)|^2\). Thus the ground-state wavefunction \(\psi_0\) is actually determined by solving a nonlinear Schrödinger equation. We will show that this approximation generally captures the physics of the large \(N\) limit; this is in contrast to the case of repulsive bosons in one dimension, for which the interaction terms must be treated more carefully \([8]\).

The solution to Eq.(3) is

\[
\psi_0(x) = \sqrt{\frac{(N-1)\alpha}{4}} \frac{1}{\cosh((N-1)\alpha x/2)} \tag{4}
\]

where \(\alpha = mW/\hbar^2\); the single particle energy is \(\epsilon = -\alpha(N - 1)^2W/8\). This has the implications for the many-body problem that there can be a state that is localized in the sense that it is unlikely that any particle be found far from the center of mass, and provides an estimate for the particle density (with the center of mass fixed at the origin) \(n(x) = N\psi(x)^2\); the corresponding ground state energy is \(E = -\alpha N(N - 1)^2W/24\).

It can be shown that there are no other bound states of Eq. (3) for the potential \(V(x)\) constructed from the ground state wavefunction. This suggests that we cannot construct approximate localized excited states of the boson molecule by symmetrizing \(\psi(x_1) \prod_{i=2}^{N} \psi_0(x_i)\) (for some appropriate choice of \(\psi\)).
The GP wavefunction is not translationally invariant, and thus violates momentum conservation. Every translation of it is a solution to the same self-consistent equation with the same energy; then by forming the linear combination \( \Psi_S(\{x_i\}) = \int \Psi(\{x_i - X\}) dX \) we can restore this symmetry.

**II. THE EXACT WAVEFUNCTION**

For the case \( N = 2 \), the wavefunction can be found by changing to relative coordinates, giving a problem equivalent to a single particle and a fixed potential well. The (unnormalized) ground state wavefunction is

\[
\Psi_2(x_1, x_2) = \exp\left(-\frac{1}{2} \alpha |x_1 - x_2|\right)
\]

where \( \alpha = mW/\hbar^2 \); the corresponding energy is \( E_2 = -\hbar^2 \alpha^2 / 4m = -mW^2/4\hbar^2 \). For \( x_1 \neq x_2 \) the delta function vanishes, and the wavefunction is an eigenfunction of the kinetic energy operator; for a bound state this is the product of exponential functions with real argument. The potential generates the discontinuity in the derivative of \( \Psi \) at the crossing point \( x_1 = x_2 \). These two properties hold for all \( N \), so that we can write down the general (unnormalized) wavefunction as

\[
\Psi_N(x_1, \ldots, x_N) = \exp\left(-\frac{\alpha}{2} \sum_{i<j} |x_i - x_j|\right)
\]

For the sector \( x_1 \leq x_2 \leq \ldots \leq x_N \) this can also be written in the form

\[
\Psi_N = \exp((1 - N)\alpha x_N/2 + (3 - N)\alpha x_{N-1}/2 + \ldots + (N - 1)\alpha x_1/2)
\]

In view of the exchange symmetry of bosons, this completely describes the wavefunction. The ground state energy is proportional to the sums of the squares of the coefficients of \( x_i \) in the argument of the exponential; explicitly,

\[
E_N = -(N^3 - N)\alpha W/24 = -(N^3 - N)mW^2/24\hbar^2
\]

This agrees with the GP result only in leading order in \( N \).

**III. THE SINGLE PARTICLE DENSITY**

The implications of the wavefunction are more clearly revealed when reduced to the probability that there is a particle at position \( x \) relative to the center of mass. For the case \( N = 2 \), there can only be a particle at \( x \) if the other is at \(-x\), and then the probability is proportional to the square of the wavefunction:

\[
P_2 = 2\alpha \exp(-2\alpha |x|)
\]

This has been normalized so that the integral over all \( x \) gives \( N = 2 \).
For larger $N$ we integrate over the unconstrained degrees of freedom; for example for $N = 3$ the probability of finding a particle at $x > 0$ is proportional to

$$\int_{-x/2}^{x} \Psi^2(-x - x_2, x_2, x) dx_2 + \int_{x}^{\infty} \Psi^2(-x - x_3, x, x_3) dx_3$$

(10)

where the integrals describe the case that it is particle 3 or particle 2 that is at $x$ (particle 1 is necessarily in the region $x < 0$). The resulting normalized probability distribution is

$$P_3(x) = 3 \cdot 2 \alpha \left[ \exp(-3\alpha|x|) - \frac{1}{2} \exp(-6\alpha|x|) \right] = 3 \cdot 2 \alpha \left[ z - \frac{1}{2} z^2 \right]$$

(11)

where in the second representation we have introduced the abbreviation $z = \exp(-N\alpha|x|)$. In a similar way $P_N$ can be constructed for other small $N$. The results for $N \leq 7$ suggest the general expression (given previously by Yoon and Negele [9])

$$P_N(x) = \alpha \frac{N!}{\prod_{n=1}^{N-1} (n!)^{\alpha}} \exp(-nN\alpha|x|)$$

(12)

This has been normalized so that the integral over all $x$ gives $N$. The density at $x = 0$ is $P_N(0) = N^2(N - 1)/(4N - 6)$. An interesting feature of the distributions is revealed when we represent them as a power series in $|x|$; the coefficients of $|x|^n$ vanish when $n$ is odd and less than $2N - 3$. Thus the discontinuity in slope at $x = 0$ that is present in $P_2$ is replaced by a discontinuity in a much higher derivative for larger $N$ (see footnote 7). This property is a demonstrable consequence of the representation (12); in fact, combined with the assumption that $P_N$ is a polynomial in $z$ of order $(N - 1)$, this is sufficient to determine the form of $P_N$ up to normalization.

In the limit of large $N$, Eq. (12) reduces to

$$P_N(x) \approx N^2\alpha \sum_{n=1}^{N-1} (-1)^{n+1} nN!N! \frac{n!}{(N + n - 1)!(N - n - 1)!} \exp(-nN\alpha|x|)$$

(13)

which has form similar to the GP result $P_N(x) = \frac{(N-1)^2\alpha}{4} \sech^2((N - 1)\alpha x/2)$. Figure 1 shows $(1/N^2\alpha)P_N(x)$ as a function of $N\alpha x$, for various $N$.

We may also characterize $P_N(x)$ through its moments. Starting from (12) it can be shown that

$$<x^2> = \frac{1}{N} \int_{-\infty}^{\infty} x^2 P_N(x) dx = \sum_{M=1}^{N-1} \frac{2}{\alpha^2 N^2 M^2} \approx \frac{\pi^2}{3\alpha^2 N^2}$$

(14)

$$<x^4> = \sum_{M=1}^{N-1} \sum_{P=1}^{N-1} \frac{12}{\alpha^4 N^4 M^2 P^2} + \sum_{M=1}^{N-1} \frac{12}{\alpha^4 N^4 M^4} \approx \frac{7\pi^4}{15\alpha^4 N^4}$$

(15)

The GP theory would give $<x^2> = \frac{\pi^2}{3\alpha^2(N-1)^{\frac{3}{2}}}$ (and similarly for $<x^4>$) – they agree at large $N$, but the exact result approaches the asymptotic limit from below, while GP approaches from above.
IV. GREEN FUNCTION AND MOMENTUM DISTRIBUTION

The single-particle Green function $G_N$ is calculated from the wavefunction by constructing the product $\Psi(x, x_2, x_3, \ldots x_N)\Psi^*(0, x_2, x_3, \ldots x_N)$ and integrating out the spectator coordinates $x_2, x_3, \ldots, x_N$. Explicit construction of the $G_N$ for $N \leq 6$ suggests the result

$$G_N(x) = \frac{g_N}{2N} \sum_{m=1}^{N} \left\{ 2 + \alpha|x| [N^2 - 1 + 4K(m)] \right\} z^{K(m)}$$

(16)

where $w = \exp(-\alpha|x|)$ and $K(m) = [N^2 - 1 - (N + 1 - 2m)^2]/4$. With the choice $g_N = 1$, $G_N(x)$ is normalized so that $G_N(0) = 1$; a physically more meaningful normalization would be to choose $\int_{-\infty}^{\infty} G_N(x) dx = 1$, but we have not succeeded in finding the closed form representation for the corresponding $g_N$. Since $K(N + 1 - m) = K(m)$, the sum contains every term twice, except for $m = (N + 1)/2$ when $N$ is odd.

In the large $N$ limit, $K(m) \approx (N - 1)(2m - 1)/2$, and then

$$G_N \approx N\alpha x/2 \sinh(N\alpha x/2) = \frac{1}{2} \int_{-\infty}^{\infty} \psi_0(x + y)\psi_0(y) dy$$

(17)

which is the Green function that one would construct from the translationally invariant GP wavefunction $\Psi_S$.

The momentum distribution is the Fourier transform of $G_N$

$$G_N(k) = \frac{1}{2N} \sum_{m=1}^{N} \left\{ \frac{\alpha K}{\alpha^2 K^2 + k^2} + \frac{\alpha^2 K^2 - k^2}{[\alpha^2 K^2 + k^2]^2} [N^2 - 1 - 4K]\right\}$$

(18)

where $k$ is the wavevector. Figure 2 gives a graph of $N\alpha G_N(k)$ versus $k/N\alpha$, for various $N$. As in the case of the repulsive boson system \[\text{[1]}\], the momentum distribution is smooth: there is no Bose condensation. The width of the momentum distribution is set by the parameter $\alpha$, so that the momentum distribution for the noninteracting case ($\alpha = 0$) is attained in a natural way. In a highly localized wavefunction we would hardly expect to find long-range off-diagonal order!

V. TWO-POINT CORRELATION FUNCTION

The two-point correlation function is calculated from the squared wavefunction by choosing one of the particles to be $x_i = 0$ and another to be at $x_j = x$ (in all possible ways), and integrating out all other $\{x_i\}$. We have chosen to normalize $C_N(x)$ so that the integral over all $x$ gives unity. It proved harder to analyze, because its representation is more irregular: for example,

$$C_6(x) = \frac{\alpha}{30} \left[ -110w^5 + 64w^8 + 81w^9 + \alpha|x| (400w^5 + 256w^8) \right]$$

(19)

where again $w = \exp(-\alpha|x|)$. Based on the explicit construction of $C_N$ for $N \leq 7$, we find

$$C_N(x) = \frac{\alpha}{2N(N - 1)} \sum_{m=1}^{N-1} \left\{ [(10K(m) - 2N^2)K(m) + \alpha|x| ([N^2 - 4K(m)]K(m))^2\right\} w^{K(m)}$$

(20)
where \( K(m) = mN - m^2 \). Since \( K(N - m) = K(m) \), the sum contains every term twice, except for \( m = N/2 \) when \( N \) is even. The special value at \( x = 0 \) (which is the probability of having two particles at the same place) is \( C_N(0) = (N + 1)/6 \). Figure 3 gives a graph of \( C_N(x)/\alpha N^2 \) for various \( N \). In the limit of large \( N \), we may approximate \( N^2 \gg K(m) \) in the prefactors and then \( K(m) \approx Nm \), with the result

\[
C_N(x) \approx \frac{\alpha}{4N} \left\{ N\alpha |x| \frac{\cosh(N\alpha x/2)}{\sinh^3(N\alpha |x|/2)} - \frac{2}{\sinh^2(N\alpha x/2)} \right\} 
\]

(21)

The structure factor is given by the Fourier transform of \( C_N(x) \):

\[
C_N(k) = \frac{\alpha}{N(N-1)} \sum_{m=1}^{N-1} K(m)^2 \left\{ \frac{[10K(m) - 2N^2]}{k^2 + K(m)^2} - \frac{[N^2 - 4K(m)][K(m)^2 - k^2]}{[k^2 + K(m)^2]^2} \right\} 
\]

(22)

VI. EXCITED STATES

In this section we will show that for any \( N \) there is only one localized state with zero total momentum. There are other states of negative energy, but these can all be interpreted as uncorrelated smaller molecules.

For indistinguishable bosons we need only specify the wavefunction for the sector \( x_1 \leq x_2 \leq \ldots \leq x_N \), and in the interior of this region (where no two coordinates are equal), the Hamiltonian operator reduces to the kinetic energy. The bound eigenstates of the kinetic energy have the form

\[
\Psi(\{x_i\}; \{k_i\}) = \exp(\sum k_i x_i),
\]

(23)

and the energy is determined to be \( E = -\sum_{i=1}^{N-1} \hbar^2 k_i^2 / 2m \). To be normalizable it is necessary that \( \sum_{i=1}^{N} k_i = 0 \) (otherwise a uniform translation of all the particles could lead to indefinite growth of \( \Psi \) ). The wavefunction for the interacting system is a linear combination of degenerate functions of this form. At the sector boundaries (where \( x_j = x_{j+1} \) for some \( j \)), the interaction gives rise to a discontinuity in the derivative of the wavefunction, which implies

\[
(\partial/\partial x_{j+1} - \partial/\partial x_j)\Psi(\{x_i\})|_{x_{j+1}=x_j} = -\alpha \Psi(\{x_i\})|_{x_{j+1}=x_j}
\]

(24)

This must hold for arbitrary choices of the remaining \( N-2 \) variables; then in the sum of terms of the form (23) the only terms that are coupled by (24) are those for which the lists \( \{k_i\} \) differ only at \( k_j \) and \( k_{j-1} \) — but then the two sum constraints on the \( \{k_i\} \) ensure that there are only two such lists, which differ by having the values for \( k_j \) and \( k_{j-1} \) interchanged. Thus the general form of the wavefunction would appear to be constructable from a single list \( \{k_i\} \) (which we will take to be ordered, so that \( k_i > k_j \) for all \( i < j \)) in the form

\[
\Psi(\{x_i\}) = \sum_P C_P \exp(\sum_{i=1}^{N} x_i k_{P(i)}),
\]

(25)

where the first sum is over all permutations of \( N \) objects, and \( P(i) \) is the \( i^{th} \) member of the permuted list. The boundary condition (24) implies relations among the coefficients \( C_P \)
\[(\alpha - k_{P(j)} + k_{P(j+1)})C_P = - (\alpha - k_{Q(j)} + k_{Q(j+1)})C_Q \equiv - (\alpha + k_{P(j)} - k_{P(j+1)})C_Q \quad (26)\]

(It should be noted that the permutations \(P\) and \(Q\) are related so that \(P(j) = Q(j+1)\) and \(P(j+1) = Q(j)\)).

The foregoing differs only slightly from the case of bosons with repulsive delta-potential interactions \([1]\) – the main difference is that the \(k_i\) are real instead of purely imaginary. However, the remaining boundary conditions are different: for repulsive interactions, the wavefunction is delocalized and must be confined within a periodic box, while for attractive interactions, the space can be infinite if the wavefunction itself is localized.

The relevant (and interesting) condition is that \(\Psi(\{x_i\})\) should become exponentially small if the extremal particle at \(x_N\) is moved to large positive \(x\), or if the particle at \(x_1\) is moved to large negative \(x\). This requires that \(k_{P(1)}\) be positive and \(k_{P(N)}\) be negative, for every term in \((25)\) that has nonzero coefficient. The sum itself is over all permutations, which certainly will generate terms in which the \(k\)'s have the wrong sign; but the coefficients will vanish (according to \((26)\)) for all permutations such that in the list \(\{k_{P(i)}\}\) it happens there are members \(k_{P(i)}\) and \(k_{P(j)}\) such that \(i < j\) and \(k_{P(j)} = k_{P(i)} - \alpha\). The ground state wavefunction is a simple example of the working of this rule: the ordered list is of the form of a sequence \((k_1, k_1 - \alpha, k_1 - 2\alpha, k_1 - 3\alpha, \ldots)\) and every possible permutation of it gives rise to a vanishing coefficient.

The ground state is not the only possibility: we could have a list which is made of several distinct sequences, so that in one of its permutations it takes the form \((k_1, k_1 - \alpha, \ldots k_a - n_a\alpha, k_b, k_b - \alpha, \ldots k_b - n_b\alpha, k_c, k_c - \alpha \ldots)\). This gives some freedom in the choice for the starting elements \(k_p\) and sublist lengths \(n_p\); this generates the wavefunction for an excited state of the molecule. However, it does not represent a localized state. Suppose we simultaneously displace the particles \(\{x_i: i = 1, 2, \ldots, n_a + 1\}\) a large distance to negative values. If \(\sum_{i=1}^{n_a+1} k_i < 0\), this term will become exponentially large, giving a nonnormalizable wavefunction. However, if \(\sum_{i=1}^{n_a+1} k_i > 0\) there will be a different permutation of the list in which this sublist is at the end, again giving a nonnormalizable wavefunction when these particles are moved to large positive values. The remaining possibility is \(\sum_{i=1}^{n_a+1} k_i = 0\) – but now the wavefunction remains finite if it is separated into two widely separated pieces, one of which contains \(n_a + 1\) particles: this describes states in which the particles have formed several separate and uncorrelated molecules.

In the foregoing argument we have assumed that the \(\{k_i\}\) are real. Allowing them to be complex does not change the situation much: the argument above implies that the \(k_i\) having a real part must be organizable into sublists as above, all having the same imaginary part; each sublist represents a separated molecule, now with finite momentum. From this point of view we can readily see that when two molecules collide, nothing happens – they pass through each other leaving each undisturbed \([9]\).

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[10] It’s a little surprising that there is any singularity, since placing one particle at the center of mass would not seem to be significantly different from placing it nearby. However, for this special position the configurations with differing numbers of particles to right and left of the origin (for $N$ even, all configurations have this property) are equivalent and coupled by the possibility of moving another particle from one side to the other.

Figure Caption
FIGURES

FIG. 1. Particle density distribution. Here are displayed $P_N(x)/\alpha N^2$ as a function of $N\alpha x$, for $N = 2, 3, 4, 5, 10, \text{ and } \infty$. The cusp in $P_2$ at $y = 0$ is replaced by discontinuities in the higher derivatives for other $N$.

FIG. 2. The single-particle momentum distribution. Here are displayed $N\alpha G_N(k)$ as a function of $k/\alpha N$, for $N = 2, 3, 4, 5, 6, \text{ and } 50$. 

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FIG. 3. The two-point correlation function. Here are displayed $C_N(x)/\alpha N^2$ as a function of $N\alpha x$, for $N = 2, 3, 4, 5, \text{ and } 6.$