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The Bose Molecule in One Dimension

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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.

KEY WORDS: One dimension; boson; Green function; momentum distribution; pair distribution; structure factor.

1. 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.

This system has recently found an experimental realization in a ^7Li vapor[4,5] 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. In this system the Li atoms are bosons[6] with an interaction that can be attractive, resulting in a collapse.[7–9] In this context, the boson molecule is called a "bright soliton."

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The wavefunction $\Psi\{x_i\}$ is an extremum 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. It can be given exactly in closed form[2][3]:

$$\Psi_N(x_1, \ldots, x_N) = \exp(-(\alpha/2) \sum_{i<j} |x_i - x_j|) \tag{2}$$

where $\alpha = mW/\hbar^2$. When the particle positions x_i are distinct, the delta function vanishes, and the wavefunction is an eigenfunction of the kinetic energy operator; for a bound state with zero total momentum this is the product of exponential functions with real argument. The potential generates a discontinuity in the derivative of Ψ at the crossing points $x_i = x_j$. In view of the exchange symmetry of bosons, we can restrict our attention to the ordered sector $x_1 \leqslant x_2 \leqslant \cdots \leqslant x_N$ (and we shall do so in what follows). Then the wavefunction takes the form

$$\Psi_N = \exp((1-N)\alpha x_N/2 + (3-N)\alpha x_{N-1}/2 + \cdots + (N-1)\alpha x_1/2). \tag{3}$$

This wavefunction is localized in the sense that the probability is small to have any two particles far apart; however, the location of the molecule is unspecified, as it must be to have zero total momentum. The wavefunction is given in unnormalized form and would require continuum normalization. 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,[3]

$$E_N = -(N^3 - N)\alpha W/24 = -(N^3 - N)mW^2/24\hbar^2. \tag{4}$$

Previous study of this model has produced three notable results:

*McGuire,[2] in addition to describing the wavefunction (2), showed that the molecule has the interesting property that in a collision between a single particle and a N-1 particle bound state, the particle is scattered without exciting the molecule.

*Yang[10] extended this to a general statement about the S-matrix for the system.

*Calogero and Degasperis[11] compared the exact solution to the results of treating this problem using the Gross-Pitaevskii (GP)[12] approximation, showing that they agree well in the large N limit (in contrast,

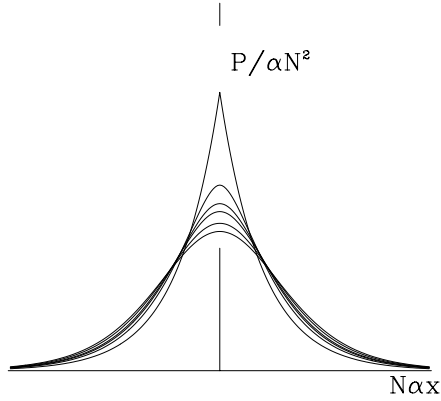

Fig. 1. Particle density distribution. Here are displayed $P_N(x)/\alpha N^2$ as a function of $N\alpha x$, for $N = 2, 3, 4, 5, 10$, and ∞. The cusp in P_2 at y = 0 is replaced by discontinuities in the higher derivatives for other N.

for the case of repulsive bosons in one dimension, the interaction terms must be treated more carefully).[13] They also determined the particle density relative to the center of mass, in the form

$$P_N(x) = \alpha \sum_{n=1}^{N-1} (-1)^{n+1} \frac{n(N!)^2}{(N+n-1)!(N-n-1)!} \exp(-nN\alpha|x|). \tag{5}$$

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. This is illustrated in figure 1, which shows $(1/N^2\alpha)P_N(x)$ as a function of $N\alpha x$, for various N.

2. GREEN FUNCTION AND MOMENTUM DISTRIBUTION

The single-particle Green function G_N is calculated from the wavefunction by constructing the product $\Psi(X, x_1, x_2, \ldots x_{N-1})\Psi^*(Y, x_1, x_2, \ldots x_{N-1})$ and integrating out the spectator coordinates $x_1, x_2, \ldots, x_{N-1}$. It is of interest because its Fourier transform is the momentum distribution, which is a directly measurable property; it is in this function that we would look for the signature of off-diagonal long-range order (we don't find it, which is the expected result).

In this section we will derive the result (previously conjectured[14] from the form of G_N for small N)

$$G_N(x) = \frac{g_N}{2N} \sum_{j=0}^{N-1} \{2 + \alpha|x|[N^2 - 1 - 4S(j)]\} w^{S(j)} \tag{6}$$

where $w = \exp(-\alpha|x|)$ and

$$S(j) = [N^2 - 1 - (N - 1 - 2j)^2]/4. \tag{7}$$

With the choice $g_N = 1$, $G_N(x)$ is normalized so that $G_N(0) = 1$; a physically more meaningful normalization is to choose $\int_{-\infty}^{\infty} G_N(x)dx = 1$, but the corresponding g_N does not have a simple expression. Since $S(N+1-j) = S(j)$, the sum contains every term twice, except for $j = (N+1)/2$ when N is odd.

The momentum distribution is the Fourier transform of G_N

$$G_N(k) = \frac{1}{2N} \sum_{j=0}^{N-1} \{2 \frac{\alpha S(j)}{\alpha^2 S(j)^2 + k^2} + \frac{\alpha^2 S(j)^2 - k^2}{[\alpha^2 S(j)^2 + k^2]^2} [N^2 - 1 - 4S(j)]\alpha\} \tag{8}$$

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,[1] the momentum distribution is smooth: there is no Bose condensation. In a highly localized wavefunction we would hardly expect to find *long-range* off-diagonal order! The width of the momentum distribution is set by the

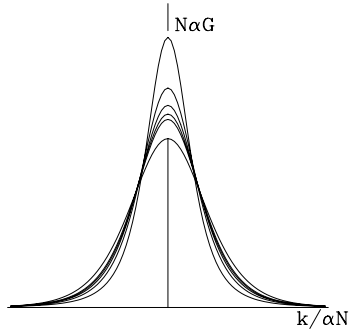

Fig. 2. The single-particle momentum distribution. Here are displayed $N\alpha G_N(k)$ as a function of $k/\alpha N$, for $N = 2, 3, 4, 5, 6,$ and 50.

parameter α, so that the momentum distribution for the noninteracting case ($\alpha = 0$) is attained in a natural way.

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

$$G_N(x) \approx N\alpha x/2 \sinh(N\alpha x/2) = \frac{1}{2}\int_{-\infty}^{\infty} \psi(x+y)\psi(y)dy \tag{9}$$

where $\psi(x) = \sqrt{\frac{1}{4}N\alpha}\cosh^{-1}(N\alpha x/2)$ is the single-particle wavefunction that results from the GP approximation.[11] This relationship can understood physically as follows: The GP wavefunction $\Psi(\{x_i\}) = \prod_i \psi(x_i)$ is not translationally invariant, and thus violates momentum conservation. However, 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. Construction of the Green function from this wavefunction leads to (11) in the large-N approximation.

The derivation of Eq.(6) is as follows, for the case that N is even. There are $(N+1)N/2$ ways for the chosen coordinates $X < Y$ to be interpolated into the ordered list of coordinates, so that $x_m \leqslant X \leqslant x_{m+1}$ and $x_n \leqslant Y \leqslant x_{n+1}$, with $0 \leqslant m \leqslant n \leqslant N-1$ (this includes the cases $X < x_1$ and $x_{N-1} < Y$). Each case is a partition that divides the list of particle coordinates into three subsets. The Green function is the sum of the integrals over all of these cases, and thus takes the form

$$G_N(X,Y) = \sum_{m=0}^{N-1}\sum_{n=m}^{N-1} I_m(X)e^{k_{m+1}X}J_{m+1,n}(X,Y)e^{k_{n+1}Y}K_{n+1}(Y), \tag{10}$$

where $k_m = (N+1)/2 - m$ (we temporarily are using a length scale such that $\alpha = 1$), and I, J, and K represent multiple integrals over the three subsets. The functions I and K can be found by doing the integrals in order, starting from x_1 or x_N:

$$\begin{aligned} I_m &= \int_{-\infty} dx_1 \int dx_2 \cdot \int^X dx_m \ \exp\left(2\sum_{i=1}^{m} k_i x_i\right) \\ &= \frac{(N-1-m)!}{m!(N-1)!}e^{m(N-m)X} \end{aligned} \tag{11}$$

and

$$K_{n+1} = \int_Y dx_{n+1} \int dx_{n+2} \cdots \int^{\infty} dx_{N-1} \ \exp\left(2 \sum_{i=n+1}^{N-1} k_{i+1} x_i\right)$$
$$= \frac{n!}{(N-1-n)!(N-1)!} e^{-(n+1)(N-1-n)Y}, \tag{12}$$

where the notation specifies that these are integrals over the sectors $-\infty \leqslant x_1 \leqslant x_2 \leqslant \cdots \leqslant x_m \leqslant X$ and $Y \leqslant x_{n+1} \leqslant \cdots \leqslant x_{N-1} \leqslant \infty$, respectively. Note that these factors are related by the parity transformation $X \to -Y$, $m \to N-1-n$, $n \to N-1-m$, $I_m(X) \to K_{n+1}(Y)$. Since we plan to normalize G_N separately, the factors of $(N-1)!$ can be omitted from I_m and K_n.

Defining $p_j = k_j + k_{j+1} = N - 2j$, the middle term is

$$J_{m+1,n}(X, Y) = \int_X dx_{m+1} \cdots \int^Y dx_n \exp\left(\sum_{j=m+1}^{n} p_j x_j\right) \tag{13}$$

This will be treated as three cases: (I) $0 \leqslant m \leqslant n \leqslant N/2-1$; (II) $N/2 \leqslant m \leqslant n \leqslant N-1$; (III) $0 \leqslant m \leqslant N/2-1$ and $3/2 \leqslant n \leqslant N-1$. Figure 3 gives a diagram showing how these are related.

*Case I: $0 \leqslant m \leqslant n \leqslant N/2-1$

The $J_{m,n}$ are related by recursion relations

$$J_{m+1,n+1}(X, Y) = \int_X^Y J_{m+1,n}(X, z) e^{p_{n+1} z} dz, \tag{14}$$

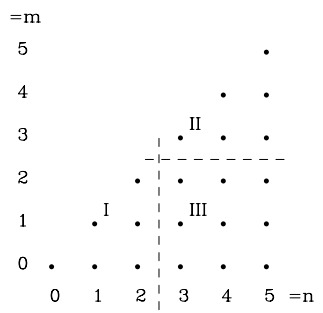

Fig. 3. The three cases, for $N = 6$. Each black dot represents a term in the sum (10); the dashed lines partition these into the three cases.

which implies

$$J_{m+1,n}(X,Y) = \sum_{j=m}^{n} (-1)^{m-j} P_{m+1,j} Q_{j+1,n} e^{(j-m)(N-1-j-m)X+(n-j)(N-1-j-n)Y}, \quad (15)$$

where

$$P_{m+1,j} = \frac{(N-1-2j)!}{(N-1-j-m)!(j-m)!} \quad (16)$$

$$Q_{j+1,n} = \frac{(N-2-j-n)!}{(N-2-2j)!(n-j)!}. \quad (17)$$

In fact, substituting Eq. (15) into Eq. (14) we find that the integrands are all exponential functions, and that the upper limit of the integral provides all of the terms for $J_{m,n+1}$ except for the very first ($j=m$) term, which can be inferred from the requirement that $J_{m,n}(X,Y)$ vanish for $X \to Y$, or by consideration of the recursion relation relating $J_{m+1,n}$ to $J_{m,n}$.

Now substitute this result and the representations (11) and (12) for the integrals $I_m(X)$ and $K_{n+1}(Y)$ into Eq. (10). This gives a representation for the contribution $G_I(X,Y)$ from this case in the form of a triple sum over the indices m, n, and j. The dependence on X and Y is purely in terms of factors of the form $\exp(S_j(X-Y))$. The sum on the index m can be done with the aid of a case of the Chu-Vandermonde identity (see Appendix),

$$\sum_{m=0}^{j} (-1)^m \frac{(N-m)!}{m!(N-m-j)!(j-m)!} = 1, \quad (18)$$

to give

$$G_I(X,Y) = \sum_{j=0}^{N/2-1} (-1)^j (N-1-2j) e^{S(j)(X-Y)} \sum_{n=j}^{N/2-1} \frac{n!(N-2-j-n)!}{(N-1-n)!(n-j)!}. \quad (19)$$

*Case II $N/2 \leqslant m \leqslant n \leqslant N-1$

This case can be treated in a way similar to case I; however, it is simpler to note that the mathematical expressions for region I and II actually are the same, with the similarity obscured by having chosen a direction in which to number the coordinates. Replacing $j \to N-1-j$, $m \to N-1-n$,

$n \to N-1-m$, $X \to -Y$, $Y \to -X$ interchanges the two regions. This implies $G_I(X,Y) = G_{II}(X,Y)$.

*Case III $0 \leqslant m \leqslant N/2-1$ and $N/2 \leqslant n \leqslant N-1$

Here we run into a difficulty. An expression can be given for $J_{m+1,n}$ having the same form as Eq. (15), but some of the factors entering into the denominators of the coefficients $P_{m+1,j}$ and $Q_{j+1,n}$ are zero, requiring that a limit be taken. This occurs because there are combinations of the k_j that vanish, and then the corresponding integrand in J is not an exponential function: it is a constant! Integrating this is easy enough, but treating it as a special case complicates the bookkeeping. The simplest way to manage the problem is to do the integral over $x_{N/2}$ last, making use of a different recursion relation:

$$J_{m+1,n}(X,Y) = \int_X^Y J_{m+1,N/2-1}(X,z) J_{N/2+1,n}(z,Y) dz \tag{20}$$

(note that $p_{N/2} = 0$). Now we can use the result (15) for the first factor $J_{m+1,N/2-1}(X,z)$ which belongs to Case I and is a sum of terms that are all exponentially increasing in z, and the corresponding result for Case II for the second factor, which is a sum of terms that are all exponentially decreasing in z. As before, upon substituting the resulting expressions into Eq. (10) to find the contribution to the Green function, we discover that the sums on m and n can be done explicitly. Then

$$\begin{aligned} G_{III}(X,Y) = \int_X^Y dz \sum_{j=0}^{N/2-1} \sum_{k=N/2}^{N-1} (-1)^{j+k+1} (N-1-2j)(2k+1-N) \\ \times \exp\left[\frac{1}{2}(N-1)(X-Y) + j(N-1-j)(X-z) \right. \\ \left. + k(N-1-k)(z-Y) \right]. \end{aligned} \tag{21}$$

It is useful to replace $k \to N-1-k'$. The resulting expression can be integrated term by term; the terms $j = k'$ are the ones that have no z dependence and must be treated separately. The result is

$$G_{III} = \sum_{j=0}^{N/2-1} (N-1-2j)^2 (Y-X) e^{S(j)(X-Y)}$$

$$+\sum_{j=0}^{N/2-1}\sum_{k=0,k\neq j}^{N/2-1}(-1)^{j+k}(N-1-2j)(2k+1-N)$$
$$\times\frac{e^{S(j)(X-Y)}-e^{S(k)(X-Y)}}{(N-1-k)k-(N-1-j)j}. \tag{22}$$

The Green function is the sum of G_I, G_{II}, and G_{III}. It has the form

$$G(X-Y)=\sum_{j=0}^{N/2-1}[(N-1-2j)^2(Y-X)+2(N-1-2j)D_j]e^{S(j)(X-Y)}, \tag{23}$$

where D_j is given by

$$D_j=(-1)^j\sum_{n=j}^{N/2-1}\frac{n!(N-2-j-n)!}{(N-1-n)!(n-j)!}$$
$$+\sum_{k=0,k\neq j}^{N/2-1}(-1)^{j+k}[\frac{1}{N-1-k-j}-\frac{1}{k-j}]. \tag{24}$$

Some of the terms in the last sum cancel each other (compare the summand for $k=p$ and $k=2j-p$). Furthermore, there is an identity (see Appendix)

$$\sum_{n=j}^{N/2-1}\frac{n!(N-2-j-n)!}{(N-1-n)!(n-j)!}=-\sum_{k=j+1}^{N-1-j}(-1)^{k+j}\frac{1}{k}; \tag{25}$$

substituting this into Eq. (24) cancels all of the remaining terms, with just one term left over! All of Eq. (24) collapses into the result $D_j=1/(N-1-2j)$. Adjusting the normalization gives Eq. (6).

The case that N is odd has to be treated separately, but the derivation is quite similar. Because we are now integrating over an even number of internal coordinates $x_1,\ldots,x_{N-1}$, there is no particular "middlemost" coordinate to leave til last, with the result that the expression corresponding to Eq. (20) is less symmetric. However, the intermediate results (11), (12), (15), and (18) remain valid; Eq. (25) continues to hold, except that the upper limit of the sum on the right should be $(N-3)/2$. We note that in the result (6) the summand takes the same values for j and $N-1-j$, allowing a trivial simplification of the result.

3. TWO-POINT CORRELATION FUNCTION

The two-point correlation function is calculated from the squared wavefunction (which gives the N-particle density) 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 $\{x_i\}$. It is a readily measurable property of the ^7Li bright soliton.

In this section we will derive the result (previously conjectured[14] from the form of G_N for small N)

$$C_N(x) = \frac{\alpha}{2N(N-1)} \sum_{m=1}^{N-1} \{[(10S(m) - 2N^2]S(m) + \alpha|x|[N^2 - 4S(m)]S(m)^2\} w^{S(m)}, \tag{26}$$

where $w = \exp(-\alpha|x|)$ and

$$S(m) = mN - m^2. \tag{27}$$

Since $S(N-m) = S(m)$, the sum contains every term twice except for $m = N/2$ when N is even. The function $C_N(x)$ is normalized so that the integral over all x gives unity. The value at $x = 0$ is $C_N(0) = (N+1)/6$ – this tells us something about the relative probability that two particles are at the same place. Figure 4 gives a graph of $C_N(x)/\alpha N$ for various N.

In the limit of large N, we may approximate $N^2 \gg S(m)$ in the prefactors and then $S(m) \approx Nm$, with the result

$$C_N(x) \approx \frac{\alpha}{4N} \left\{ N\alpha|x| \frac{\cosh(N\alpha x/2)}{\sinh^3(N\alpha|x|/2)} - \frac{2}{\sinh^2(N\alpha x/2)} \right\}. \tag{28}$$

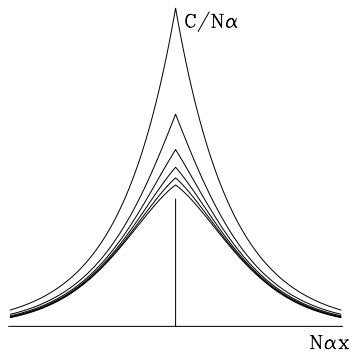

Fig. 4. The two-point correlation function. Here are displayed $C_N(x)/\alpha N$ as a function of $N\alpha x$, for $N = 2, 3, 4, 5,$ and 6.

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

$$C_N(k) = \frac{\alpha}{N(N-1)} \sum_{m=1}^{N-1} S(m)^2 \left\{ \frac{[10S(m) - 2N^2]}{k^2 + S(m)^2} - \frac{[N^2 - 4S(m)][S(m)^2 - k^2]}{[k^2 + S(m)^2]^2} \right\}. \tag{29}$$

The derivation of Eq. (26) is similar to the derivation of the Green function. Assuming N to be odd, the correlation function can be written as a sum

$$C_N(X, Y) = \sum_{m=0}^{N-2} \sum_{n=m}^{N-2} I_m(X) e^{2k_{m+1}X} J_{m+1,n}(X, Y) e^{2k_{n+1}Y} K_{n+2}(Y), \tag{30}$$

where $k_m = (N+1)/2 - m$. The function I_m is the same as previously, and K_{n+1} can be constructed from it by the parity transformation $X \to -Y$, $m \to N-2-n$, $I_m \to K_{n+1}$. The discussion of the function $J_{m+1,n}$ is similar to that above, with the only difference being that now $p_j = 2k_{j+1} = N - 1 - 2j$, so that N should be replaced by $N-1$ in (15), (16), and (17). As in the case of the Green function, we will divide the computation of C_N into three cases: (I) $0 \leqslant m \leqslant n \leqslant (N-3)/2$; (II) $(N-1)/2 \leqslant m \leqslant n \leqslant N-2$; (III) $0 \leqslant m \leqslant (N-3)/2$ and $(N-1)/2 \leqslant n \leqslant N-2$. Figure 3 can be read as a diagram showing how these regions are related for the case $N = 7$.

*Case I: $0 \leqslant m \leqslant n \leqslant (N-3)/2$

Here and in case III we need to calculate

$$\begin{aligned} &\sum_{m=0}^{j} I_m(X) e^{2k_{m+1}X} J_{m+1}(X, Y) \\ &\quad = \sum_{j=0}^{n} \sum_{m=0}^{j} \frac{(N-1-m)!}{m!} \frac{(N-2-2j)!(-1)^{m-j}}{(N-2-j-m)!(j-m)!} Q_{j+1,n} \\ &\qquad \times e^{(N^2-(2j-N+2)^2)X/4} e^{(n-j)(N-2-j-n)Y} \\ &\quad = \sum_{j=0}^{n} \frac{(j+1)(N-1-j)(N-2-2j)(N-3-j-n)!}{(n-j)!} \\ &\qquad \times e^{(N^2-(2j-N+2)^2)X/4} e^{(n-j)(N-2-j-n)Y}, \end{aligned} \tag{31}$$

wherein the Chu-Vandermonde identity (see Appendix) has been used. Then

$$C_I = \sum_{j=0}^{n} (j+1)(N-1-j)(N-2-2j)e^{S_{j+1}(X-Y)} \times \sum_{n=j}^{(N-3)/2} \frac{(N-2-j-n)!(n+1)!}{(n-j)!(N-n-2)!}. \tag{32}$$

*Case II $(N-1)/2 \leqslant m \leqslant n \leqslant N-2$

This case is related to Case I by the parity transformation, and gives an equal contribution to the correlation function.

*Case III $0 \leqslant m \leqslant (N-3)/2$ and $(N-1)/2 \leqslant n \leqslant N-2$

For this case we calculate $J_{m+1,n}$ by doing the integral over $x_{(N-1)/2}$ last, as was done for the Green function. Substituting (31) twice,

$$\begin{aligned} C_{III} = & \sum_{j=0}^{(N-3)/2} (N-2-2j)^2(j+1)^2(N-1-j)^2(Y-X)e^{S_{j+1}(X-Y)} \\ & + \sum_{j=0}^{(N-3)/2} \sum_{k=0,k\neq j}^{(N-3)/2} \\ & \times \frac{(N-2-2j)(j+1)(N-1-j)(N-2-2k)(k+1)(N-1-k)}{(N-2-j-k)(k-j)} \\ & \times (-1)^{j+k}(e^{S_{j+1}(X-Y)} - e^{S_{k+1}(X-Y)}). \end{aligned} \tag{33}$$

With the aid of the identity (see Appendix)

$$\begin{aligned} & \sum_{n=j}^{(N-3)/2} \frac{(N-3-j-n)!(n+1)!}{(n-j)!(N-2-n)!} + (N-1)/2 \\ & \quad = -(j+1)(N-j-1) \sum_{k=2j+1}^{N-2} \frac{(-1)^k}{k-j} \end{aligned} \tag{34}$$

and some algebra, these results can be combined to give Eq. (26). The derivation for the case of even N is expected to be similar; the form (26) has been checked for the cases $N = 2, 4,$ and 6.

4. 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. This argument was alluded to but not given explicitly by McGuire[2] and Yang.[10] They did show that the S-matrix is not singular, but this could have meant that there are states that cannot be excited in a collision; this interpretation becomes tenable when one realizes that the Bethe Ansatz implies the existence of as many conserved quantities as there are particles.

For indistinguishable bosons we need only specify the wavefunction for the sector $x_1 \leqslant x_2 \leqslant \cdots \leqslant x_N$; 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

$$\Psi(\{x_i\}; \{k_i\}) = \exp(\sum k_i x_i), \tag{35}$$

and the energy is determined to be $E = -\sum_{i=1}^{N} \hbar^2 k^2 / 2\mathrm{m}$. 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 Ψ). 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[1]

$$(\partial/\partial x_{j+1} - \partial/\partial x_j)\Psi(\{x_i\})_{|x_{j+1}=x_j} = -\alpha \Psi(\{x_i\})_{|x_{j+1}=x_j}. \tag{36}$$

This must hold for arbitrary choices of the remaining $N-2$ variables; then in the sum of terms of the form (35) the only terms that are coupled by Eq. (36) 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

$$\Psi(\{x_i\}) = \sum_P C_P \exp(\sum_{i=1}^{N} x_i k_{P(i)}), \tag{37}$$

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 (36) implies

relations among the coefficients C_P

$$\begin{aligned}(\alpha - k_{P(j)} + k_{P(j+1)})C_P &= -(\alpha - k_{Q(j)} + k_{Q(j+1)})C_Q \\ &\equiv -(\alpha + k_{P(j)} - k_{P(j+1)})C_Q \end{aligned} \tag{38}$$

(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 condition defining a bound state 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 Eq. (37) 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 Eq. (38)) 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 $(k_1, k_1 - \alpha, k_1 - 2\alpha, k_1 - 3\alpha, \dots)$ 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 $(k_1, k_1 - \alpha, \dots k_a - n_a\alpha, k_b, k_b - \alpha, ..k_b - n_b\alpha, k_c, k_c - \alpha \dots)$. 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 $\{x_i : i = 1, 2, .., n_a + 1\}$ 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.[15]

APPENDIX. FACTORIAL SUMS

Our work in several places is based upon the Chu-Vandermonde identity[16] in the form

$$\sum_{p=0}^{q}(-1)^p\frac{(N+q-p)!}{p!(q-p)!(N+q-r-p)!}=\frac{r!N!}{q!(r-q)!(N+q-r)!}, \tag{39}$$

wherein we have assumed $N>r\geqslant q$; for $N>q>r$ the right-hand side vanishes. This identity can be used to show that Eq. (15) vanishes for $X=Y$ (completing the task of solving the recursion relation (14); Eq. (18) is the special case $r=q=j$; and in arriving at Eq. (31) we have chosen $q\to j$, $r\to j+1$, $N\to N-j-1$.

The identity Eq. (25) is not well known, but can be derived as follows: use the Beta function[19] to write

$$\begin{aligned}\mathcal{S}&=\sum_{p=0}^{M}\frac{(j+p)!(2M-p)!}{(2M+j+1-p)!p!}\\&=\int_0^1\sum_{p=0}^{M}\frac{(2M-p)!}{p!(2M-2p)!}t^{j+p}(1-t)^{2M-2p}dt\\&=\int_0^1\sum_{p=0}^{M}\sum_{k=0}^{2M-2p}\frac{(-1)^k(2M-p)!}{p!k!(2M-2p-k)!}t^{j+p+k}dt.\end{aligned} \tag{40}$$

Now perform the integration over t, and rearrange the double sum into a sum over k and $K=p+k$:

$$\mathcal{S}=\sum_{K=0}^{2M}\frac{(-1)^K}{K+j+1}\sum_{p=0}^{min(K,2M-K)}(-1)^p\frac{(2M-p)!}{p!(K-p)!(2M-K-p)!}$$

$$= \sum_{K=0}^{2M} \frac{(-1)^K}{K+j+1}, \tag{41}$$

where Eq. (39) has been used: for $K \leqslant M$, the sum over p is the case $q = K$, $r = K$, $N = 2M - K$; for $K > M$, the sum over p is the case $q = 2M - K$, $r = 2M - K$, $N = K$. When applying Eq. (39), each of these inner sums turns out to be 1.

Thus we obtain the identity

$$\mathcal{S} = \sum_{p=0}^{M} \frac{(j+p)!(2M-p)!}{(2M+j+1-p)!p!} = \sum_{K=0}^{2M} \frac{(-1)^K}{K+j+1}. \tag{42}$$

Equation (25) is a special case of Eq. (42): set $M = \frac{N}{2} - (j+1)$ in Eq. (42), and then shift the index of summation up by j on the LHS and by $j+1$ on the RHS. Finally, take $p = n$ and $K = k$.

The identity Eq. (34) is an immediate consequence of

$$\sum_{p=0}^{M} \frac{(j+1+p)!(2M-p)!}{(2M+j+1-p)!p!} = (M+1) - (j+1)(2M+j+2) \sum_{K=0}^{2M-1} \frac{(-1)^K}{K+j+2}. \tag{43}$$

To obtain Eq. (34) from Eq. (43), first shift the index of summation up by j on the LHS and by $2j+2$ on the RHS. Add and subtract the $K = 2j+1$ term on the RHS. Finally, set $M = \frac{N}{2} - j - \frac{3}{2}$, $p = n$, $K = k$, and simplify.

To prove Eq. (43), first note that the $p = M$ term on the LHS is 1. An analysis similar to that in Eqs. (40)–(41) above applied to the $p = 0$ to $p = M - 1$ terms on the LHS of Eq. (43) yields the double sum

$$\sum_{K=0}^{2M-1} \frac{(-1)^K}{K+j+2} \sum_{p=0}^{min(K,2M-1-K)} (-1)^p \frac{(2M-p)!}{p!(K-p)!(2M-K-1-p)!} = \sum_{K=0}^{2M-1} (-1)^K \frac{(K+1)(2M-K)}{K+j+2}, \tag{44}$$

where Eq. (39) has been used: for $K < M$, the sum over p is the case $q = K$, $r = K+1$, $N = 2M - K$; for $K \geqslant M$, the sum over p is the case

$q = 2M - 1 - K$, $r = 2M - K$, $N = K + 1$. When applying (39), the K-th inner sum was $(K+1)(2M-K)$.

We further simplify Eq. (44) by making use of the partial fraction identity (in K):

$$\frac{(K+1)(2M-K)}{K+j+2} = (2M+j+1) - K - \frac{(j+1)(2M+j+2)}{K+j+2}. \qquad (45)$$

Applying Eq. (45) termwise to the RHS of Eq. (44) produces three sums. The first is 0, the second is M, and the third is the RHS of Eq. (43) minus $(M+1)$. This completes the proof of Eq. (43).

The identities (42) and (43) can be extended to more complicated formulas where $(j+p)!$ and $(j+1+p)!$ on the left-hand-sides are replaced by $(j+b+p)!$, for integral values of b other than 0 and 1. However, these two cases (arising naturally in Eq. (25) and (34)) are by far the simplest.

The above derivation of Eq. (25) and (34) can also be done in terms of hypergeometric series notation.

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