Three-body exclusion principle, duality mapping, and exact ground state of a harmonically trapped, ultracold Bose gas with three-body hard-core interactions in one dimension

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Motivated by previous suggestions that three-body hard-core interactions in lower-dimensional ultracold Bose gases might provide a way for creation of non-Abelian anyons, the exact ground state of a harmonically trapped 1D Bose gas with three-body hard-core interactions is constructed by duality mapping, starting from an N-particle ideal gas of mixed symmetry with three-body nodes, which has double occupation of the lowest harmonic oscillator orbital and single occupation of the next N – 2 orbitals. It has some similarity to the ground state of a Tonks-Girardeau gas, but is more complicated. It is proved that in 1D any system of N ≥ 3 bosons with three-body hard-core interactions also has two-body soft-core interactions of generalized Lieb-Liniger delta function form, as a consequence of the topology of the configuration space of N particles in 1D, i.e., wave functions with only three-body hard core zeroes are topologically impossible. This is in contrast with the case in 2D, where pure three-body hard-core interactions do exist, and are closely related to the fractional quantized Hall effect. The exact ground state is compared with a previously-proposed Pfaffian-like approximate ground state, which satisfies the three-body hard-core constraint but is not an exact energy eigenstate. Both the exact ground state and the Pfaffian-like approximation imply two-body soft-core interactions as well as three-body hard-core interactions, in accord with the general topological proof.

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If an ultracold atomic vapor is confined in a de Broglie wave guide with transverse trapping so tight and temperature so low that the transverse vibrational excitation quantum is larger than available longitudinal zero point and thermal energies, the effective dynamics becomes one-dimensional (1D) [1, 2]. 3D Feshbach resonances [3] allow tuning to the neighborhood of 1D confinement-induced resonances [1, 2], where the 1D interaction is very strong, leading to short-range correlations, breakdown of effective-field theories, and emergence of highly-correlated N-body ground states. In the case of spinless or spin-polarized bosons with 1D zero-range Lieb-Liniger (LL) [3] delta function repulsion \( g_2 \delta(x_j - x_k) \) with coupling constant \( g_2 \to +\infty \), the Tonks-Girardeau (TG) gas, the exact N-body ground state was determined in 1960 by a Fermi-Bose (FB) mapping to an ideal Fermi gas [4], leading to “fermionization” of many properties of this Bose system, as recently confirmed experimentally [7, 8].

Under conditions of ultracold gas experiments, the 1D two-body interaction Hamiltonian is usually well-approximated by the zero-range LL potential \( V_2 = g_2 \sum_{1 \leq j < k \leq N} \delta(x_j - x_k) \), and the dimensionless coupling constant measuring its strength is \( \gamma_2 = mg_2/\hbar^2 \) where \( n \) is the 1D number density. \( \gamma_2 \ll 1 \) is the Gross-Pitaevskii regime and \( \gamma_2 \gg 1 \) is the TG regime. A three-body zero-range interaction potential generalizing the LL-interaction is \( V_3 = g_3 \sum_{1 \leq j < k < \ell \leq N} \delta(x_j - x_k)\delta(x_j - x_\ell) \), and its dimensionless coupling constant is \( \gamma_3 = mg_3/\hbar^2 \). Note that \( \gamma_3 \) is independent of the density, whereas \( \gamma_2 \) has the density in the denominator. Hence, attainment of the two-body TG limit \( \gamma_2 \gg 1 \) requires very low density or very large \( g_2 \), the reason why attainment of this limit is so difficult and the experiments [7, 8] were tours de force. This suggests that attainment of the three-body hard-core limit \( \gamma_3 \gg 1 \) may be easier than reaching the TG limit. Although three-body collisions are rare at the usual densities of ultracold gases, the magnitude of the three-body scattering length does not depend on density.

Laughlin’s wave function [5] for the ground state of a 2D electron gas in a magnetic field in the lowest Landau level is \( \exp(-\frac{1}{\ell^2} \sum_{j=1}^{N} |z_j^2|) \prod_{1 \leq j < k \leq N} (z_j - z_k)^\nu \) where \( \nu \) is an odd integer. It is an ansatz describing quasiparticles of fractional charge \( e/\nu \) in the fractional quantum Hall effect. Here \( z_j = x_j + iy_j \) are complex position coordinates in the \((x, y)\) plane, \( \ell^2 = \hbar/m\omega_c \), and \( \omega_c \) is the cyclotron frequency. In the limit of infinitely strong interaction it is known [10, 11] that the exact ground state for even \( N \) is a closely related Pfaffian-like wave function \( \Psi_0 = \hat{S}_{\mathrm{T}4} \exp(-\frac{1}{\ell^2} \sum_{j=1}^{N} |z_j^2|) \prod_{j<k} (z_j - z_k)^\nu \prod_{j<k|l} (z_j - z_k - z_\ell)^2 \) where \( \hat{S}_{\mathrm{T}4} \) symmetrizes over all ways of subdividing the \( N \) particles into two subsets of \( N/2 \) each. It describes particles with 2D three-body hard-core interactions, since \( \Psi_0 \) vanishes when \( z_j = z_k = z_\ell \) for all choices \( j < k < \ell \). The strong similarity between the Laughlin wave function and the 1D TG ground state \( \psi_{BG0}(x_1, \ldots, x_N) = \)

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where $Q_i = x_i / x_{\text{osc}}$ with $x_{\text{osc}} = \sqrt{\hbar/m\omega}$ the oscillator length, suggests a possible close connection with the problem of three-body hard-core interactions in 1D, motivating Paredes et al. [13] to suggest a similar Pfaffian-like state as an ansatz for the 1D ground state. It was previously suggested [11][14] that the fractional quantum Hall effect in 2D might lead to a class of quasiparticles obeying non-Abelian anyon statistics, with potentially important applications to creation of topologically protected qubits for quantum computation, and very recently experimental evidence for such quasiparticles has been found [15]. Although no way is currently known for producing such quasiparticles in 1D, this is further motivation for exploring connections between three-body interactions in 2D and those in 1D, as suggested in [13].

Paredes et al. [13] assume that $N$ is even, and construct an approximate ground state by dividing the $N$ particles into two subsets of $\frac{N}{2}$ each, assuming that each of these two is in an $\frac{N}{2}$-particle TG ground state, taking the product of these two states, finally restoring the required bosonic symmetry over all $N!$ permutations by symmetrizing over all ways of choosing two subsets of $\frac{N}{2}$ particles from all $N$. They assumed that the $N$ bosons were trapped on a ring, thus requiring the ring-periodic TG ground state [6]. However, the TG ground state in a harmonic trap is much simpler [12]. With that choice the ansatz of [13] is $\Psi_{\text{ansatz}} = \exp(-\sum_{j=1}^{N} m\omega x_j^2/2\hbar)S[\prod_{i<j}^{N/2} |x_i - x_j|][\prod_{k<l}^{N/2} |x_k - x_l|]$ where $S$ is the symmetrizer described above. The similarity with the above 2D Pfaffian-like state is evident. This state vanishes when $x_j = x_k = x_\ell$ for all $1 \leq j < k < \ell \leq N$, because any such choice requires that at least two of these three coordinates, say $x_p$ and $x_q$, lie in the same subset, giving a vanishing factor $|x_p - x_q|$ with $x_p = x_q$. However, it is not an energy eigenstate. Numerical calculations described in [13] suggest that its error does not exceed 10%. In the remainder of this paper the exact ground state with three-body hard-core interactions will be constructed by combining a three-body exclusion principle with a duality mapping generalizing that of [6].

Three-body exclusion principle and ideal gas with three-body nodes: The key to finding the exact ground state of a 1D Bose gas with three-body hard-core interactions is a three-body exclusion principle and its application to generation of three-body nodes in an ideal gas of mixed symmetry. The Pauli exclusion principle requires that all $N$-particle wave functions of a system of fermions must be totally antisymmetric under all permutations of its particle coordinates $X_j$, where $X_j$ includes both the spatial position and any discrete internal quantum numbers. For a system of particles without internal quantum numbers, one consequence is that all allowed wave functions vanish if two or more particles have the same spatial position. Although a corollary of this is that allowed wave functions vanish if three particles are at the same point, this is an utterly trivial consequence. A much weaker requirement is that allowed wave functions must vanish if three or more particles are at the same point, with no restriction on the wave function if two are at the same point. This defines a "three-body exclusion principle", and is the starting point for the determination herein of the exact ground state of bosons with three-body hard-core interactions in 1D. The Hamiltonian $H_0$ of $N$ identical particles in 1D with no interparticle interactions in a harmonic trap consists of only the kinetic energy and the trap potential:

$$H_0 = \sum_{j=1}^{N} \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + \frac{1}{2} m\omega^2 x_j^2 \right). \tag{1}$$

Its eigenstates are trapped ideal gas states, and the first goal here is to find ideal gas states of mixed symmetry satisfying the three-body exclusion principle. The single-particle energy eigenstates in the trap are the orbitals $\phi_n(x) = c_n \exp(-m\omega^2 x^2/2\hbar)H_n(x/x_{\text{osc}})$ where $H_n$ are the Hermite polynomials and $c_n$ is a normalization constant. Start from an unsymmetrized orbital product state $\Psi_{0U}$ with two particles in the lowest orbital and one in each of the remaining $N-2$ lowest orbitals:

$$\Psi_{0U} = \phi_0(x_1)\phi_0(x_2)\phi_1(x_3)\cdots\phi_{N-2}(x_N). \tag{2}$$

It is an eigenstate of $H_0$ with energy

$$E_0 = \left( \frac{1}{2} + \frac{1}{2} + \frac{3}{2} + \cdots + \frac{2N-3}{2} \right)\hbar\omega = \frac{1}{2}(N^2-2N+2)\hbar\omega, \tag{3}$$

and this will remain true if its $N$ arguments $(x_1, \ldots, x_N)$ are permuted in any way, and for all linear combinations of such products. Our goal is to choose linear combinations summing to a mixed-symmetry "model state" $\Psi_{0M}$ which satisfies the three-body exclusion principle. This requirement is satisfied by choosing coefficients $\pm 1$ in such a way that $\Psi_{0M}$ is the sum of $N$ terms, each of which is the product of the lowest orbital $\phi_0(x_j)$, with $j$ ranging from 1 to $N$, and a Slater determinant with the remaining $N-1$ atoms occupying each of $\phi_0, \phi_1, \ldots, \phi_{N-2}$ once:

$$\Psi_{0M}(x_1, \ldots, x_N) = \sum_{j=1}^{N} \phi_0(x_j)\text{det}_{(n,k=0,1),k\neq j}^{(N-1,N)} \phi_n(x_k). \tag{4}$$

The antisymmetry of each Slater determinant ensures that if more than two particles are at the same point $x_j = x_k = x_\ell = x$, $\Psi_{0M}$ will vanish, i.e. this $(N-3)$-dimensional hyperline is a three-body node of $\Psi_{0M}$. If $x_j = x_k = x$ and $x_\ell$ is in the neighborhood of $x$, then $\Psi_{0M}$ changes sign as $x_\ell$ passes through $x$, i.e., it is locally but not globally antisymmetric about that point. Next, note that since $H_0(x) = 1$, each of the prefactors...
\( \phi_0(x_j) \) reduces to \( \exp(-m\omega x_j^2/2\hbar) \). Finally, elementary row and column operations and van der Mond’s theorem can be applied as they were in \[12\] to the derivation of the ground state of the harmonically trapped TG gas, to reduce each Slater determinant to a Bijl-Jastrow product of \((N - 1)(N - 2)/2\) factors \((x_k - x_l)\). The final result is

\[
\Psi_{0M}(x_1, \ldots, x_N) = \exp\left(-\sum_{j=1}^{N} m\omega x_j^2/2\hbar\right) \times \prod_{j=1}^{N} (x_k - x_l) \tag{5}
\]

where an irrelevant normalization factor has been dropped.

**Evaluation of \( \Psi_{0B} \) by duality mapping:** A wave function \( \Psi_{0B} \) with Bose symmetry (totally symmetric), which is an eigenstate of \( \hat{H}_0 \) with eigenvalue \( E_0 \) of Eq. \[5\] when all \( N \) coordinates are different, and vanishes when any three are equal, can be found by a duality mapping generalizing that used to find the TG ground state \[12\]. Each locally antisymmetric factor \((x_k - x_l)\) can be converted into an absolute value \(|x_k - x_l|\) by multiplication by a signum function \( \text{sgn}(x_k - x_l) = +1(-1), x_k - x_l > 0(< 0) \), yielding

\[
\Psi_{0B}(x_1, \ldots, x_N) = \exp\left(-\sum_{j=1}^{N} m\omega x_j^2/2\hbar\right) \times \prod_{j=1}^{N} |x_k - x_l| \tag{6}
\]

Since each factor \( \text{sgn}(x_k - x_l) \) is constant except for a sign change at \( x_k = x_l \), it follows that except at collision points \( x_k = x_l \), \( \Psi_{0B} \) is still an eigenstate of \( \hat{H}_0 \) with eigenvalue \( E_0 \). It is the desired exact ground state with three-body hard-core interactions. It is instructive to write it out explicitly for \( N = 3 \) and \( N = 4 \). For \( N = 3 \) Eq. \[6\] reduces to

\[
\Psi_{0B}(x_1, x_2, x_3) = \exp\left(-\sum_{j=1}^{3} m\omega x_j^2/2\hbar\right) \times (|x_2 - x_3| + |x_1 - x_3| + |x_1 - x_2|) \tag{7}
\]

which obviously vanishes if \( x_1 = x_2 = x_3 \). For \( N = 4 \) one finds

\[
\Psi_{0B}(x_1, \ldots, x_4) = \exp\left(-\sum_{j=1}^{4} m\omega x_j^2/2\hbar\right) \times (|x_2 - x_3||x_2 - x_4||x_3 - x_4| + |x_1 - x_3||x_1 - x_4||x_3 - x_4| + |x_1 - x_2||x_1 - x_4||x_2 - x_4| + |x_1 - x_2||x_1 - x_3||x_2 - x_3|) \tag{8}
\]

which vanishes if \( x_2 = x_3 = x_4 \) or \( x_1 = x_3 = x_4 \) or \( x_1 = x_2 = x_4 \) or \( x_1 = x_2 = x_3 \).

**Implicit two-body interactions:** For consistency a three-body hard-core potential term \( V_3 = \lim_{g_3 \to +\infty} g_3 \sum_{1 \leq j < k \leq N} \delta(x_j - x_k) \delta(x_j - x_l) \) should be added to \( \hat{H}_0 \) to exhibit the three-body hard-core interaction. A subtlety that appears to have been missed previously is that in 1D, the existence of three-body hard-core interactions automatically generates two-body soft-core interactions as well. This is not true in 2D, but in 1D it is an unavoidable consequence of the topology of the configuration space, and holds for any many-boson wave function satisfying the three-body hard-core constraint, whether the exact ground state of Eq. \[10\] or an approximate ground state such as the Pfaffian-like ansatz of \[13\], and it holds for excited states as well. To see this, note that the three-body hard-core constant region \( x_j = x_k = x_l \) is an \((N - 1)\)-dimensional hyperplane which is the common intersection of the three \((N - 1)\)-dimensional hyperplanes \( x_j = x_k, x_j = x_l, x_k = x_l \), and these hyperplanes divide the configuration space into disjoint regions. On the other hand, in 2D the coordinates \( z_j \) are complex numbers in the \((x,y)\) plane, the region \( z_j = z_k = z_l \) has dimension \( 2N - 6 \), and the two-body collision regions each have dimension \( 2N - 2 \), also hyperlines which are easily circumvented, and there is an exact ground state with only three-body hard cores, realized by a state of Pfaffian form \[10, 11\]. Returning to the 1D case, suppose, for example that \( x_1 = x_2 < x_3 < x_4 \), and we wish to realize a three-body hard-core interaction at \( x_1 = x_2 = x_3 \). Then the particle originally at \( x_3 \) must be moved to the left across the particle at \( x_4 \), crossing the hyperplane \( x_3 = x_4 \). This generates a finite two-body interaction at \( x_3 = x_4 \), since local Bose symmetry about this plane requires that the wave function \( \Psi \) satisfy \( \Psi(x_1, x_2, x_3, x_3 + \epsilon, x_5, \ldots) = \Psi(x_1, x_2, x_3, x_3 - \epsilon, x_5, \ldots) \) for infinitesimal \( \epsilon \). So long as \( \partial\Psi(x_1, x_2, x_3, x_3 + \epsilon, x_5, \ldots)/\partial\epsilon \) does not vanish, this requires that \( \partial\Psi(x_1, x_2, x_3, x_4, x_5, \ldots)/\partial x_4 \) change sign at \( x_4 = x_3 \), implying that there will be a cusp on the hyperplane \( x_3 = x_4 \). The same proof applies, with the obvious changes of arguments, in the neighborhood of every hyperplane \( x_3 = x_4 \). This is the typical behavior for eigenstates of a Hamiltonian containing a LL two-body interaction term \[2\] \( V_2 = g_2 \sum_{1 \leq j < k \leq N} \delta(x_j - x_k) \delta(x_j - x_l) \), where \( g_2 \) is finite so long as \( \Psi \) does not vanish there, true only for a two-body hard-core interaction (TG limit). \( g_2 \) can be determined in the usual way by integrating Schrödinger’s equation from \( x_j = x_k \) to \( x_j = x_k^+ \), or, perhaps more simply, by noting which Dirac delta function terms are generated when the kinetic energy operator acts on the absolute value factors in \( \Psi \), and noting that these must be cancelled by like delta function terms in a two-body interaction Hamiltonian \( V_2 \) which must be added to \( \hat{H}_0 \) to cancel them, in order that \( E_0 \Psi \).
contain no delta functions. Since the value of $\Psi$ on the hyperplane $x_j = x_k$ depends on all the other coordinates, $g_2$ is not constant as in the usual LL interaction, but depends on all the coordinates: $g_2 = g_2(x_1, \cdots, x_N)$. For the case $N = 3$, one finds after some algebraic reduction

$$g_2(x_1, x_2, x_3) = \frac{\hbar^2}{2m} \left( |x_1 - x_2| + |x_1 - x_3| + |x_2 - x_3| \right)^{-1}.$$  

(9)

As $x_3$ approaches the hyperplane $x_1 = x_2$, $g_2 \to +\infty$, showing that the three-body hard-core interaction is already implied by the dependence of $g_2$ on $x_3$, and the same argument applies for the other two hyperplanes. The complexity of the explicit expression increases rapidly with $N$, but $g_2$ is always of the form $\frac{\hbar^2}{2m}$ times an expression $\frac{\alpha}{D}$, where the denominator $D$ is just $\Psi_{0B}$ of Eq. (6) with the exponential prefactor omitted, and the numerator $\alpha$ is a sum of products of factors $|x_p - x_q|$ of degree one less than the denominator. It approaches $+\infty$ as any three particles approach the same point.

Comparison of exact ground state and Pfaffian-like approximation: The Pfaffian-like approximate ground state of Paredes et al. [13] is defined only for even $N$, and is obtained by subdividing the set of $N$ particles into two subsets of $\frac{N}{2}$ each, assuming that each of these subsets is in its TG ground state, taking the product of these two $\frac{N}{2}$-particle states, and restoring total Bose symmetry by summing over all ways of selecting $\frac{N}{2}$ from $N$. They assumed ring geometry, necessitating more complicated ring-periodic TG states, but here the simpler case of harmonic trapping is assumed. For the simplest case $N = 4$ the result is

$$\Psi_{0Pf}(x_1, \cdots, x_4) = \exp(-\sum_{j=1}^{4} m\omega x_j^2 / 2\hbar) \times \left( |x_1 - x_2| |x_3 - x_4| + |x_1 - x_3| |x_2 - x_4| + |x_1 - x_4| |x_2 - x_3| \right),$$  

(10)

which is to be compared with the exact ground state, Eq. (8). The Pfaffian-like state is simpler, being built from products of two factors $|x_p - x_q|$ as compared with products of three in (10), but (8) is exact whereas (10) is not an energy eigenstate, although it does vanish if any three particles are at the same point. It is easy to see that the Pfaffian-like state leads to soft-core LL two-body interactions depending on all four coordinates when the kinetic energy Hamiltonian acts on the absolute values, just as the exact ground state does, in accord with the previous topological proof.

Discussion and Outlook: The exact ground state of a harmonically trapped system of $N \geq 3$ bosons in 1D with three-body hard-core interactions was found by duality mapping from an ideal gas of mixed symmetry with three-body nodes. It was found to have two-body soft-core interaction cusps as well, and it was shown that this is an inescapable consequence of the topology of the configuration space of a system of $N \geq 3$ bosons in 1D with three-body hard-core interactions. In view of previous suggestions of a possible connection between three-body hard-core interactions and non-Abelian anyons with potential applications to creation of topologically-protected qubits for quantum computation, it seems worthwhile to look for ways of producing three-body hard-core interactions in a 1D ultracold Bose gas. This might be facilitated by the fact that the dimensionless coupling constant for three-body interactions in 1D is a density-independent ratio $\gamma_3 = mg_3/\hbar^2$, so higher densities could be used than are required to reach the two-body hard-core limit $\gamma_2 = mg_2/\hbar^2 \gg 1$, which requires low densities $n$.

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