Static and Dynamic Properties of Trapped Fermionic Tonks-Girardeau Gases

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We investigate some exact static and dynamic properties of one-dimensional fermionic Tonks-Girardeau gases in tight de Broglie waveguides with attractive p-wave interactions induced by a Feshbach resonance. A closed form solution for the one-body density matrix for harmonic trapping is analytically analyzed in terms of its natural orbitals, with the surprising result that for odd, but not for even, numbers of fermions the maximally occupied natural orbital coincides with the ground harmonic oscillator orbital and has the maximally allowed fermionic occupancy of unity. The exact dynamics of the trapped gas following turnoff of the p-wave interactions are explored.

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The spin-statistics theorem, according to which identical particles with integer spin are bosons whereas those with half-integer spin are fermions, breaks down if the particles are confined to one or two dimensions. Realization of this fact had its origin when it was shown by one of us [1] that the many-body problem of hard-sphere bosons in one dimension can be mapped exactly onto that of an ideal Fermi gas via a Fermi-Bose (FB) mapping. It is now known that this “Fermi-Bose duality” is a very general property of identical particles in one-dimension (1D). In recent years this subject has become highly relevant through experiments on ultracold atomic vapors in atom waveguides [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. Exploration of these systems is facilitated by tunability of their interactions by external magnetic fields via Feshbach resonances [15]. In fermionic atoms in the same spin state, s-wave scattering is forbidden by the exclusion principle and p-wave interactions are usually negligible. However, they can be greatly enhanced by Feshbach resonances, which have recently been observed in an ultracold atomic vapor of spin-polarized fermions [16]. Additional resonances, which have recently been observed in an ultracold atomic waveguide [17, 18], a regime already reached experimentally [19], and recently Granger and Blume derived an effective Hamiltonian for longitudinal scattering of two spin-aligned fermions confined in a single-mode harmonic atom waveguide [20]. It can be shown [21, 22] that in the low-energy domain the K-matrix can be reproduced, with a relative error as small as O(k^2), by the contact condition

\[ \psi_F(x_{j\ell} = 0+) = -\psi_F(x_{j\ell} = 0-) = -a_1^{F}\psi_F(x_{j\ell} = 0\pm) \]
where the prime denotes differentiation,

$$a_{1D}^F = \frac{6 V_p}{a_\perp^2} [1 + 12 (V_p/a_\perp^3)] |\zeta(-1/2, 1)|^{-1} \tag{3}$$

is the one-dimensional scattering length, $a_\perp = \sqrt{\hbar/\mu\omega_\perp}$ is the transverse oscillator length, $V_p = a_p^2 = -\lim_{k \to 0} \tan \delta_p(k)/k^3$ is the p-wave “scattering volume” \[27\], $a_p$ is the p-wave scattering length, $\zeta(-1/2, 1) = -\zeta(3/2)/4\pi = -0.2070\ldots$ is the Hurwitz zeta function evaluated at $(-1/2, 1)$ \[24\], and $\mu = m/2$ is the reduced mass. The expression \[13\] has a resonance at a negative critical value $V_p^{crit}/a_\perp^2 = -0.4009\ldots$. In accordance with \[23\], the low-energy fermionic wavefunctions are discontinuous at contact, but left and right limits of their derivatives coincide, and following Ref. \[21\] we assume the same here. For an interatomic interaction of short but nonzero range $x_0$, the fermionic relative wave function vanishes at $x_j = 0$; Eq. \[2\] refers to the $x_0 \to 0$ limit of the exterior wave function just outside the range of the interaction \[21\], \[22\].

The contact condition \[2\] is generated by the 1D interaction pseudopotential operator \[24\], \[24\].

$$\phi_{in}^F = g_{1D}^F \sum_{1 \leq j < j \leq N} \delta(x_{j+1}) \delta_j \psi \left(1/2\right) \delta(x, x + q) \psi(x)$$

where $\delta_j \psi = (1/2) \delta_{x, x + q} \psi(x)$ with effective 1D coupling constant $g_{1D}^F = \hbar^2 a_{1D}^F / \mu$. This can be compared with the 1D coupling constant $g_{1D}^B = -\hbar^2 a_{1D}^B / \mu \perp$. The dimensionless fermionic coupling constant is $\gamma_F = -mg_{1D}^B / nh^2$. Note that the density $n$ is in the numerator, whereas it is in the denominator of the bosonic analog $\gamma_B = mg_{1D}^B / nh^2$.

**Fermionic TG gas:** The fermionic TG gas regime is $\gamma_F \gg 1$ valid in the neighborhood of the resonance where the denominator of Eq. \[9\] vanishes.

The 1D scattering length is invariant under the FB mapping \[1\], \[20\], \[21\], \[22\].

$$\psi_B = A(x, \ldots, x_N) \psi$$

with $A(x_1, \ldots, x_N) = \prod_{1 \leq j < j \leq N} \text{sgn}(x_j - x_i)$ the “unit antisymmetric function” employed in the original discovery of fermionization \[1\], so we shall henceforth indicate it by $a_{1D} = a_{1D}^F = a_{1D}^B$. Since $V_p$ must be negative to achieve a resonance, the fermionic TG regime with attractive p-wave interactions $a_{1D} \to -\infty$ and $g_{1D}^F \to -\infty$ is reached as $V_p$ approaches the resonance through negative values, implying an interaction-free exterior wave function. More generally, the spin-aligned Fermi gas maps to the Lieb-Liniger Bose gas \[23\], \[23\] with fermionic and bosonic coupling constants inversely related \[21\] according to $g_{1D}^B = -\hbar^2 / \mu^2 g_{1D}^F > 0$. The corresponding dimensionless coupling constants $\gamma_B = mg_{1D}^B / nh^2 > 0$ and $\gamma_F = -mg_{1D}^B / nh^2 > 0$ satisfy $\gamma_B^2 F = 4 \gamma_F$ \[22\].

**Natural orbitals:** The N-atom ground state of the longitudinally trapped fermionic TG gas maps to the trapped ideal Bose gas ground state ($\gamma_B = 0$) for which all N atoms are Bose-Einstein condensed into the lowest HO orbital $\phi_0(x)$:

$$\psi_F(x_1, \ldots, x_N, t = 0) = A(x_1, \ldots, x_N) \prod_{j=1}^N \phi_0(x_j).$$

Since $A^2 = 1$, all properties expressible in terms of $|\psi(x)|^2$, including the density profile, are the same as those of the trapped Bose gas ground state $\prod_{j=1}^N \phi_0(x_j)$. However, properties not so expressible, such as the momentum distribution, differ dramatically, as in the case of the usual bosonic TG gas. The appropriate tool for studying such differences is the reduced one-body density matrix (OBDM) $\rho_1(x, x'; t) = N \int \psi_F(x, x_2, \ldots, x_N, t) \phi_0^*(x') \psi_F(x', x_2, \ldots, x_N) dV x_2 \cdots dV x_N$. The normalized natural orbitals satisfy $\lambda_{ji} \rho_1(x, x'; t) = 0 = u_j(x')$, with eigenfunctions $u_j(x)$, $j = 0, 1, 2, \ldots$, and eigenvalues or orbital occupations $0 \leq \lambda_j \leq 1$. For a spatially uniform bosonic TG gas of length $L$, the natural orbitals are plane waves $u_j(x) = e^{i2\pi x j / L} / \sqrt{L}$ and the distribution of occupations $\lambda_j$ reflects a momentum distribution function with low-momentum peaking and broad wings, whereas for a free Fermi gas the ground state is a filled Fermi sea with $\lambda_j = 1$, $j = 0, 1, \ldots, N - 1$, all other occupations being zero \[13\], \[14\], \[28\]. Although natural orbitals are much-used in quantum chemistry, the first application to degenerate gases is due to Dubois and Glyde \[31\].

In the case of the longitudinally trapped fermionic TG gas, the OBDM can be evaluated in closed form for all $N$ \[31\] yielding $

$$\rho_1(x, x'; t = 0) = N \phi_0(x) \phi_0(x') \left(F(x, x')\right)^{N-1}$$

where $F(x, x') = \int_{-\infty}^{\infty} \text{sgn}(x - x') \text{sgn}(x' - x') \phi_0^2(x') dV x' = 1 - \text{erf}(Q') - \text{erf}(Q)$, with erf the error function \[32\].

We have numerically diagonalized the OBDM to obtain the natural orbitals and occupations for a variety of $N$. In Figs. \[1\]a and \[b\] we show the occupations $\lambda_j$ versus orbital number $j$ for $N = 2$ and $N = 3$, respectively, as representative of our findings for even and odd numbers of atoms. (The solid line between data points is included as an aid to the eye). For $N = 2$ we see that the occupancy distribution shows a staircase structure where $\lambda_{2q} \simeq \lambda_{2q+1}$, $q = 0, 1, 2, \ldots$, the occupancies being monotonically decreasing $\lambda_j > \lambda_{j+1}$. Furthermore, the occupancy distribution extends well beyond the Fermi sea for the corresponding free Fermi gas shown as the dashed line, reflecting the strongly interacting nature of the fermionic TG gas. For $N = 3$ shown in Fig. \[1\]b a similar staircase structure is seen with the exception that $\lambda_0 = 1$, that is the natural orbital $u_0(x)$ has the maximal occupancy allowed by the exclusion principle, and $\lambda_{2q+1} \simeq \lambda_{2q+2}$, $q = 0, 1, 2, \ldots$.

The natural orbitals are structurally similar to the HO orbitals and share the property that the orbital number $j$ is equal to the number of field nodes. To examine the properties of the maximally occupied natural orbital we used a Rayleigh-Ritz variational procedure with a Gaussian trial solution $u_0(x) = \exp(-x^2/2\mu^2) / \pi^{1/4} \sqrt{\mu}$ to obtain the corresponding occupancy $\lambda_0(w)$ numerically. We have found that for odd $N$ the maximal occupancy obtained by varying $w$ is $\lambda_0(w = x_{osc}) = 1$ for $w = x_{osc}$, so that the maximally occupied natural orbital $u_0(x)$ co-
can be written in terms of the HO orbitals that serve as
the initial OBDM. Formally, the solution for the OBDM
sequence of the strong many-body correlations present in
no interactions the subsequent dynamics are a direct con-
particle HO Hamiltonian. Even though this equation has
\[ \hat{H} = \frac{\hbar^2}{2m} \nabla^2 + V(x) \]
the maximum occupancy is obtained numerically for
\( N \), an exact and surprising result. In contrast, for even
\( N \) the occupancy increasing with \( N \) but re-
remaining less that unity, and comparison of the numerical
results and Gaussian solution shows that it is an approxi-
mation less that unity, and comparison of the numerical
results and Gaussian solution shows that it is an approxi-
mation to the maximally occupied natural orbital, albeit
a very good one.

**Dynamics following turnoff of interactions:** We next
examine the *exact* dynamics of the fermionic TG gas
that ensue when the interactions are suddenly turned
off at \( t = 0 \) by detuning the external magnetic field.
For \( t < 0 \) the OBDM is given by that for the fermionic
TG gas \( \rho_1(x,x';t < 0) = \sum_j \lambda_j u_j(x)u_j(x') \). For later
times, when the interactions are turned off, the evolu-
tion of the OBDM is given by
\[ i\hbar(\partial/\partial t)\rho_1(x,x';t) = [\hat{H}(x) - \hat{H}(x')]\rho_1(x,x';t) \]
where \( \hat{H}(x) \) is the single-particle HO Hamiltonian. Even though this equation has
no interactions the subsequent dynamics are a direct con-
squence of the strong many-body correlations present in
the initial OBDM. Formally, the solution for the OBDM
can be written in terms of the HO orbitals that serve as
natural orbitals for the non-interacting gas
\[ \rho_1(x,x';t > 0) = \sum_{n,m} C_{nm} \phi_n(x)\phi_m(x')e^{-i(n-m)\omega t}, \]
where \( C_{nm} = \sum_j \lambda_j \int dxu_n(x)\phi_j(x)\int dxu_m(x)\phi_j(x) \), and the symmetry of the orbitals dictates that \( C_{nm} \) is
non-zero only for \( n \) and \( m \) both even or both odd. Thus,
the OBDM evolution following the turnoff of the interac-
tions is periodic in time with period \( T = \pi/\omega \). We have
solved the equation of motion for the OBDM numerically
to obtain the exact dynamics of the initial fermionic TG
gas, and here we present results for the evolution of the
density profile \( \rho(x,t) = \rho_1(x,x;t) \).

Figure 2(a) shows the scaled density profile \( \rho_{osc}(Q,t = T/2) \) after half a
period for \( N = 2 \) and \( N = 8 \) (dashed line), and \( N = 3 \)
and \( N = 9 \) (dashed line).

\[ \text{FIG. 1: Occupation distribution } \lambda_j \text{ versus natural orbital number } j \text{ for a) } N = 2, \text{ and b) } N = 3. \text{ In each case the dashed line shows the corresponding result for a free Fermi gas.} \]

\[ \text{FIG. 2: Scaled density profile } \rho_{osc}(Q,t = T/2) \text{ after half a period for a) } N = 2 \text{ and } N = 8 \text{ (dashed line), and b) } N = 3 \text{ and } N = 9 \text{ (dashed line).} \]
again under the action of the harmonic single particle potential, the initial condition being recovered at $t = T$.

Figure 2(b) shows the corresponding results for $N = 3$ and $N = 9$ (dashed line), and similar broadening is seen at $t = T/2$. In this case, however, a density maximum is maintained at the center of the trap. The persistence of an on-axis density peak for odd $N$ may be understood as follows: For odd $N$ the particles are symmetrically placed around the center of the trap with one particle at the center. When the interactions are turned off the particles displaced from the center will move outwards in reaction to the Fermi degeneracy pressure. However, the center particle, which is absent for even $N$, will be pinned at the center by the equal but opposite Fermi degeneracy pressures acting on it due to the displaced particles, and this maintains the on-axis density peak for odd $N$. The persistence of a central peak may also be related to the fact that for odd $N$ the maximally occupied natural orbital $u_0(x)$ for the fermionic TG gas with interactions is identical to the HO orbital $\phi_0(x)$ which serves as a natural orbital with no interactions. Thus, the scaled density profile associated with this maximally occupied orbital is given by $x_{osc}u_0(Q) = C_0u_0u_{osc}^2(0) = \exp(-Q^2)/\sqrt{\pi}$, which has a maximum on-axis, integrates to unity and represents the centrally pinned particle, and persists after the interactions are turned off. For $N = 3$ simulation in Fig. 2(b) $x_{osc}u_0(0,T/2) \simeq 0.6$, whereas $x_{osc}u_0(0) = 0.56$, showing that the central peak is largely accounted for by the maximally occupied natural orbital. For larger odd $N$ the central maximum has a larger contribution from higher natural orbitals but the peak still persists; see the dashed line in Fig. 2(b).

In summary, the OBDM of a harmonically trapped fermionic TG gas has been analyzed in terms of its natural orbitals and occupations. For an odd number of atoms the maximally occupied natural orbital was found to coincide with the single-particle HO ground state. Due to the rarity of exact results for strongly interacting systems it is important to suggest observable consequences. We have explored the exact dynamics following turnoff of the $p$-wave interactions, finding that for odd $N$ the on-axis density remains a maximum as the cloud expands due to Fermi degeneracy pressure, in contrast to even $N$ where the density develops a minimum.

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