Pairing of a harmonically trapped fermionic Tonks-Girardeau gas

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The fermionic Tonks-Girardeau (FTG) gas is a one-dimensional spin-polarized Fermi gas with infinitely strong attractive zero-range odd-wave interactions, arising from a confinement-induced resonance reachable via a three-dimensional $p$-wave Feshbach resonance. We investigate the off-diagonal long-range order (ODLRO) of the FTG gas subjected to a longitudinal harmonic confinement by analyzing the two-particle reduced density matrix for which we derive a closed-form expression. Using a variational approach and numerical diagonalization we find that the largest eigenvalue of the two-body density matrix is of order $N/2$, where $N$ is the total particle number, and hence a partial ODLRO is present for a FTG gas in the trap.

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I. INTRODUCTION

Low-dimensional systems display unusual and striking features as compared to their three-dimensional (3D) counterparts, among which are the enhanced effects of the interactions and the presence of large fluctuations which are responsible for the failure of mean-field approaches. In addition, especially in the one-dimensional (1D) case, it is possible to find exact solutions which greatly help the progress in our understanding of complex, strongly-interacting many-body systems.

Low-dimensional atomic quantum gases are one of the frontiers of the current theoretical and experimental investigations. Bosonic and fermionic atomic gases constrained to a quasi-1D geometry have already been realized experimentally by trapping atoms in two-dimensional optical lattices\textsuperscript{1, 2}. In the case of bosons the strongly-repulsive (known as Tonks-Girardeau) regime has been achieved\textsuperscript{3, 4}. This regime has been fully understood thanks to the knowledge of the exact many-body wavefunction through the mapping of the strongly repulsive, impenetrable bosons onto an ideal gas of fermions subjected to the same external potential\textsuperscript{5, 6, 7, 8}. Quite remarkably, the mapping does not hold only for the ground state, but may be extended to treat time-dependent phenomena and systems at finite temperature\textsuperscript{6, 7, 8}. In this paper we focus on the model of spin-polarized fermions interacting via strongly attractive odd-wave interactions, which are the 1D analogue of $p$-wave interactions in 3D. This regime might be experimentally reachable by exploiting the so-called confinement-induced resonances (CIR), which permit to tune the 1D coupling constant via a 3D Feshbach resonance\textsuperscript{9}. In the limit of infinitely strong attractions, known as the fermionic Tonks-Girardeau (FTG) regime, the many-body wavefunction is known exactly through an inverse Fermi-Bose mapping which allows to express the fermionic wavefunction in terms of the one of an ideal Bose gas\textsuperscript{9, 10, 11}. At the resonance point we can thus quantitatively address the question of what the structure of the ground state is, and in particular whether the fermions are paired. This contributes to the understanding of the intermediate, strongly-interacting region in the 1D equivalent of the BCS-BEC crossover for $p$-wave fermions.

In a previous work\textsuperscript{12} we have studied the issue of pairing for a homogeneous FTG gas in the thermodynamic limit. We have found that there is off-diagonal long-range order (ODLRO) in the reduced two-body density matrix, indicating a paired state. We consider here the experimentally-relevant case of a gas with a finite number of particles and subjected to a longitudinal harmonic confinement. We derive an exact analytic expression for the two-body density matrix of the trapped gas and both by variational estimates and by numerical diagonalization we show that also in the presence of the trap ODLRO persists, yielding a complex, partially paired quantum state.

II. FERMIONIC TONKS-GIRARDEAU GAS IN A LONGITUDINAL HARMONIC TRAP

We consider an atomic spin-polarized Fermi gas confined by a tight atom waveguide of which it occupies the transverse ground state. We shall henceforth assume that the level spacing in the transverse direction is much larger than all the relevant energy scales in the problem (such as chemical potential, temperature, etc.), so that the gas is effectively one-dimensional. We also consider the case of a gas subjected to a much weaker longitudinal harmonic...
confinement of frequency $\omega$. The 1D Hamiltonian is

$$\hat{H} = \sum_{j=1}^{N} \left[ -\hbar^2 \frac{\partial^2}{2m \partial x_j^2} + \sum_{1 \leq \ell \leq N} v_F^i(x_j - x_{\ell}) + \sum_j \frac{1}{2} m \omega^2 x_j^2 \right], \quad (1)$$

where $v_F^i$ is a short-range attractive two-body interaction which is specified here below. Since the spatial wave function is antisymmetric due to the spin polarization, there is no zero-range $s$-wave (delta function) interaction, but it has been shown [9, 10, 11] that a strong, attractive, and short-range odd-wave interaction (a 1D analog of 3D $p$-wave interactions) occurs in the neighborhood of the CIR. Such an interaction can be expressed through a contact condition for the relative wavefunction $\psi_F(x)$ of each pair of fermions as [13]

$$\left. \frac{1}{\psi_F(x)} \frac{d\psi_F(x)}{dx} \right|_{x=0} = -\frac{2\hbar^2}{mg_{1D}}, \quad (2)$$

where $g_{1D}^F$ is the 1D fermionic coupling constant, which can be expressed in terms of the 3D $p$-wave scattering volume [8]. The condition (2) above, together with the antisymmetry condition $\psi_F(x < 0) = -\psi_F(x > 0)$ on the relative wavefunction leads to a solution for $\psi_F(x)$ which is discontinuous at the contact point $x = 0$ but has a continuous first derivative.

The FTG gas corresponds to the negative side of the CIR, that is, the case where $g_{1D}^F \to -\infty$; in the FTG limit the first derivative of the relative wavefunction $\psi_F(x)$ equals to zero at $x = 0$. For the sake of illustration, let us consider first two particles under harmonic confinement. In the presence of such a confinement the Schroedinger equation can be solved exactly for any value of the coupling strength $g_{1D}^F$ [14]. The relative wavefunction $\psi_F(x)$ in the FTG limit takes the value $\psi_F(x > 0) = (2\pi)^{-1/4} x_{osc}^{-1/2} e^{-Q'^2/4}$ and $\psi_F(x < 0) = -(2\pi)^{-1/4} x_{osc}^{-1/2} e^{-Q'^2/4}$, where we have set $Q = x/x_{osc}$ and $x_{osc} = \sqrt{\hbar/m\omega}$.

The solution for $N = 2$ can be extended to arbitrary particle numbers $N$, so that the exact fermionic TG gas ground-state wavefunction is [9, 10]

$$\Psi_F(x_1, \ldots, x_N) = A(x_1, \ldots, x_N) \prod_{j=1}^{N} \phi_0(x_j) \quad (3)$$

with where $A(x_1, \ldots, x_N) = \prod_{1 \leq \ell \leq N} \text{sgn}(x_\ell - x_j)$ is the “unit antisymmetric function" employed in the original discovery of fermionization [9] and $\phi_0(x) = \frac{1}{x_{osc}} e^{-1/2 - Q'^2/2}$ is the ground-state orbital of the longitudinal harmonic confinement. Hence, the FTG gas is mapped through the function $A$ to the ground state of an ideal Bose gas under harmonic confinement, of which it shares all the properties that do not depend on the sign of the many-body wavefunction, such as the density profile and the spectrum of collective excitations.

III. OFF-DIAGONAL LONG-RANGE ORDER FOR A TRAPPED FTG GAS

In order to explore the pairing properties of the FTG gas we study the two-body reduced density matrix, defined as

$$\rho_2(x_1, x_2; x'_1, x'_2) = N(N-1) \int \Psi_F(x_1, x_2, \ldots, x_N) \Psi_F^*(x'_1, x'_2, \ldots, x_N) dx_3 \ldots dx_N. \quad (4)$$

As it was discussed by Yang [15], the criterion for “superconducting" off-diagonal long-range order (ODLRO) in a trapped system is that the largest eigenvalue $\lambda_1$ of the two-body density matrix is of the order of the number of particles $N$, i.e. $\lambda_1 = \alpha N$, with $0 < \alpha \leq 1$ being the pair-condensate fraction.

Using the exact form of the many-body wavefunction, the integration over $N - 2$ variables in Eq. (4) can be explicitly performed and we obtain an analytic expression for the two-body density matrix, which reads

$$\rho_2(x_1, x_2; x'_1, x'_2) = N(N-1) \text{sgn}(x_1 - x_2) \phi_0(x_1) \phi_0(x_2) \times \text{sgn}(x'_1 - x'_2) \phi_0(x'_1) \phi_0(x'_2) [G(x_1, x_2; x'_1, x'_2)]^{N-2}, \quad (5)$$

where $G(x_1, x_2; x'_1, x'_2) = 1 + \text{erf}(y_1) - \text{erf}(y_2) + \text{erf}(y_3) - \text{erf}(y_4)$, and $y_1 \leq y_2 \leq y_3 \leq y_4$ are $(Q_1, Q_2, Q'_1, Q'_2)$ in ascending order, and $Q_i = x_i/x_{osc}$.

The eigenvalues $\lambda_j$ and eigenfunctions $u_j$ of the two-body density matrix are the solutions of the integral equation

$$\int dx'_1 dx'_2 \rho_2(x_1, x_2; x'_1, x'_2) u_j(x'_1, x'_2) = \lambda_j u_j(x_1, x_2). \quad (6)$$

If $N = 2$ then $G(x_1, x_2; x'_1, x'_2) = 1$, the two-body density matrix separates trivially and has only one nonzero eigenvalue $\lambda_1 = N = 2$, with eigenfunction $u_1(x_1, x_2) = \text{sgn}(x_1 - x_2) \phi_0(x_1) \phi_0(x_2)$. For $N = 3$ we have found by numerical integration that the ansatz $u_1(x_1, x_2) = C \text{sgn}(x_1 - x_2) \phi_0(x_1) \phi_0(x_2)[1 - \text{erf}(Q_1) - \text{erf}(Q'_2)]$ satisfies the above eigenvalue equation to within 0.1% with eigenvalue $\lambda_1 = 2$ (the same as for $N = 2$), and we conjecture that these expressions are exact. For $N \geq 4$ we have numerically solved the eigenvalue equation (6) by diagonalization. The results for the largest eigenvalue are displayed in Fig. 11 for $N = 4$ to 8. The obtained values agree with the analytical expression $\lambda_1 = (N + 1)/2$ to within the computational accuracy of a few percent [10], indicating that in the trap a partial ODLRO is present. The eigenfunctions corresponding to the largest eigenvalues obtained by numerical diagonalization are shown in Fig. 12 along with the analytical eigenfunctions for $N = 2$ and 3.

We have also calculated lower bounds to $\lambda_1$ for $N = 4$ to 8 from the inequality

$$\lambda_1 \geq \frac{\int u_{\text{trial}}(X) \rho_2(X, X') u_{\text{trial}}(X') dXdX'}{\int u_{\text{trial}}^2(X) dX}, \quad (7)$$
where $X$ is a shorthand notation for $(x_1, x_2)$. In particular, we have chosen the ansatz $u_{\text{trial}}(x_1, x_2) = C \operatorname{sgn}(x_1 - x_2)\phi_0(x_1)\phi_0(x_2)[1 - \operatorname{erf}(Q_1) - \operatorname{erf}(Q_2)]^{N-2}$. As in is illustrated in Fig. 1, the results are very close to the numerical eigenvalues, indicating that the ansatz is a good guess for the exact solution. There is however some small difference, as is shown in Fig. 3 by comparing the above ansatz with the numerically determined eigenfunctions in the case $N = 4$.

Finally, it is interesting to estimate the behaviour of the two-body density matrix in the thermodynamic limit, defined as the limit $N \to \infty$, $\omega \to 0$ keeping the central density $n_0 = N\phi_0^2(0) = N\sqrt{m\omega/\pi \hbar}$ constant. In that case Eq. 4 takes the same form as in the homogeneous system 12 and hence it follows that $\rho_2(x_1, x_2; x_1', x_2') = \lambda_1 u_1(x_1, x_2)u_1(x_1', x_2')$ (apart from terms decaying exponentially with pair separation), with $\lambda_1 = N/2$ and $u_1(x_1, x_2) \propto \operatorname{sgn}(x_1 - x_2)e^{-2n_0|x_1 - x_2|}$. Hence, the estimate in the thermodynamic limit agrees to order $1/N$ with the numerical solution.

**IV. SUMMARY AND CONCLUDING REMARKS**

In summary, by estimating the largest eigenvalue of the two-body reduced density matrix we have investigated the possibility of off-diagonal long-range order for a fermionic Tonks-Girardeau gas subjected to a longitudinal harmonic confinement. The result of variational approach and numerical diagonalization together with an estimate in the thermodynamic limit is that the largest eigenvalue $\lambda_1$ is of order $N/2$, where $N$ is the particle number, and hence we find a partial ODLRO. The value $\lambda_1 \simeq N/2$ might also be interpreted as the fraction of pairs which are Bose-Einstein condensed in the onedimensional equivalent of the BCS to BEC crossover for $p$-wave fermions. The emerging picture is the one of a partially paired quantum state, where quantum fluctuations play a major role in depleting the “BEC” of pairs. The consequences of pairing remain to be explored.

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