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 [1,2]. In the case of bosons the strongly repulsive (known as the Tonks-Girardeau) regime has been achieved [3,4]. This regime has been fully understood thanks to the knowledge of the exact many body wave function through the mapping of the strongly repulsive, impenetrable bosons onto an ideal gas of fermions subjected to the same external potential [5]. 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 [6–8]. In particular, for a harmonically trapped Tonks-Girardeau gas the full dynamics induced by a sudden change of the trap frequency can be exactly solved by a scaling and gauge transformation [9], while for the general case of a trapped Lieb-Liniger gas only approximate solutions are available [10,11].

In this paper we focus on the model of spin-polarized fermions interacting via strongly attractive odd-wave interactions, which are the 1D analog of p-wave interactions in 3D. This regime might be experimentally reachable by exploiting the so-called confinement-induced resonances (CIR), which permit one to tune the 1D coupling constant via a 3D Feshbach resonance [12]. In the limit of infinitely strong attractions, known as the fermionic Tonks-Girardeau (FTG) regime, the many-body wave function is known exactly through an inverse Fermi-Bose mapping which allows one to express the fermionic wave function in terms of the one of an ideal Bose gas [12–14]. 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 to Bose-Einstein condensate (BEC) crossover for p-wave fermions.

In a previous work [15] 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 ω. The 1D Hamiltonian is

$$\hat{H}=\sum_{j=1}^{N}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_j^2}\right]+\sum_{1\leqslant j<\ell\leqslant N}v_{\mathrm{int}}^F(x_j-x_\ell)+\sum_j\frac{1}{2}m\omega^2x_j^2 \tag{1}$$

where v_{int}^F is a short-range attractive two-body interaction which is specified here below. Since the spatial wave func-

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tion is antisymmetric due to the spin polarization, there is no zero-range s-wave (δ-function) interaction, but it has been shown [12–14] 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 wave function $\psi_F(x)$ of each pair of fermions as [16]

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

where g_{1D}^F is the 1D fermionic coupling constant, which can be expressed in terms of the 3D p-wave scattering volume [12]. The condition (2) above, together with the antisymmetry condition $\psi_F(x<0)=-\psi_F(x>0)$ on the relative wave function, 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 wave function $\psi_F(x)$ equals 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 Schrödinger equation can be solved exactly for any value of the coupling strength g_{1D}^F [17]. The relative wave function $\psi_F(x)$ 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 wave function is [12,13]

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

where $A(x_1,\ldots,x_N)=\Pi_{1\leqslant j<\ell\leqslant N}\,\mathrm{sgn}(x_\ell-x_j)$ is the "unit antisymmetric function" employed in the original discovery of fermionization [5] and $\phi_0(x)=\pi^{-1/4}x_{osc}^{-1/2}e^{-Q^2/2}$ 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 wave function, 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

$$\rho_2(x_1,x_2;x_1',x_2')=N(N-1)\int\Psi_F(x_1,x_2,\ldots,x_N)\times\Psi_F^*(x_1',x_2',x_3,\ldots,x_N)dx_3\cdots dx_N. \quad (4)$$

As it was discussed by Yang [18], the criterion for "superconductive" off-diagonal long-range order in a trapped system is that the largest eigenvalue λ_1 of the two-body density matrix is of the order of the number of particles N, i.e., $\lambda_1=\alpha N$, with $0<\alpha\leqslant1$ being the pair-condensate fraction.

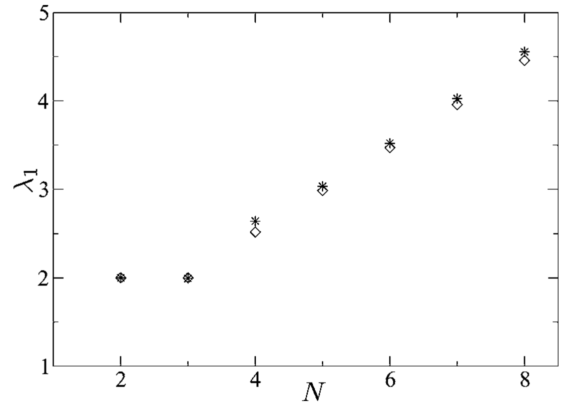

FIG. 1. Largest eigenvalue λ_1 of the two-body density matrix for a harmonically trapped fermionic TG gas at various particle numbers N from numerical diagonalization (stars) and the variational lower-bound estimate (diamonds).

Using the exact form (3) of the many-body wave function, 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

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

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

The eigenvalues λ_j and eigenfunctions $u_j(x_1,x_2)$ 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 $u_1(x_1,x_2)=\mathrm{sgn}(x_1-x_2)\phi_0(x_1)\phi_0(x_2)$. For $N=3$ we have found by numerical integration that the ansatz $u_1(x_1,x_2)=\mathcal{C}\,\mathrm{sgn}(x_1-x_2)\phi_0(x_1)\phi_0(x_2)[1-|\mathrm{erf}(Q_1)-\mathrm{erf}(Q_2)|]$ 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 $N\geqslant4$ we have numerically solved the eigenvalue equation (6) by diagonalization. The results for the largest eigenvalue are displayed in Fig. 1 for $N=4-8$. The obtained values agree with the analytical expression $\lambda_1=(N+1)/2$ to within the computational accuracy of a few percent [19], 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. 2 along with the analytical eigenfunctions for $N=2$ and 3.

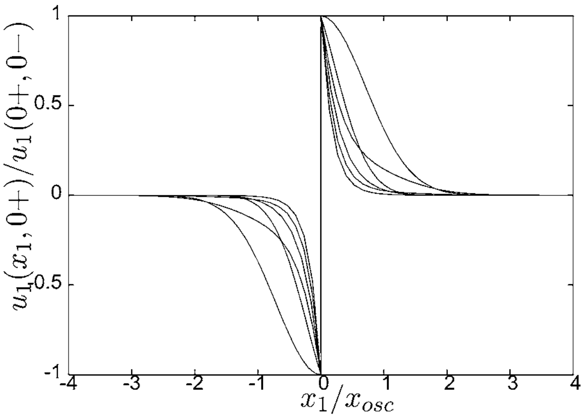

FIG. 2. Eigenfunctions of the two-body density matrix of a harmonically trapped fermionic TG gas belonging to the largest eigenvalue λ_1, for $N=2-7$ from top to bottom (when $x_1>0$).

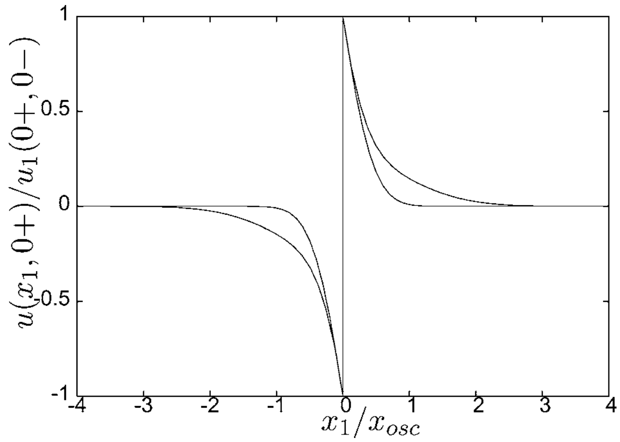

FIG. 3. Comparison of maximal eigenfunction $u=u_1$ of the two-body density matrix (upper curve when $x_1>0$) and variational ansatz $u=u_{\text{trial}}$ (lower curve when $x_1>0$) for the case $N=4$. In the case $N=3$ (not plotted) the two curves (on the same scale) would be indistinguishable.

We have also calculated lower bounds to λ_1 for $N=4-8$ from the inequality

$$\lambda_1 \geqslant \frac{\int u_{\text{trial}}(\mathbf{X})\rho_2(\mathbf{X},\mathbf{X}')u_{\text{trial}}(\mathbf{X}')d\mathbf{X}\,d\mathbf{X}'}{\int u_{\text{trial}}^2(\mathbf{X})d\mathbf{X}}, \tag{7}$$

where $\mathbf{X}$ is a shorthand notation for (x_1,x_2). In particular, we have chosen the ansatz $u_{\text{trial}}(x_1,x_2)=\mathcal{C}\,\text{sgn}(x_1-x_2)\phi_0(x_1)\phi_0(x_2)[1-|\text{erf}(Q_1)-\text{erf}(Q_2)|]^{N-2}$. As 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 behavior 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. (5) takes the same form as in the homogeneous system [15] 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 $u_1(x_1,x_2)\propto\text{sgn}(x_1-x_2)e^{-2n_0|x_1-x_2|}$. 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 λ_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 one-dimensional 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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