Pairing, Off-Diagonal Long-Range Order, and Quantum Phase Transition in Strongly Attracting Ultracold Bose Gas Mixtures in Tight Waveguides

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A model of two 1D ideal Bose gases A and B with strong odd-wave AB attractions induced by a p-wave AB Feshbach resonance is studied. The model is solved exactly by a Bose-Bose duality mapping, and it is shown that there is no A-component or B-component Bose-Einstein condensation and no AB-pair off-diagonal long-range order (ODLRO), but both AA-pair and BB-pair ODLRO. After generalization by adding even-wave AA and BB repulsions and reducing the strength of the odd-wave AB attraction by Feshbach resonance detuning, a quantum phase transition occurs between a phase with AB contact nodes and one with no such nodes.

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Strong interatomic interactions and correlations occur in ultracold gases confined in de Broglie waveguides with transverse trapping so tight that the atomic dynamics is essentially 1D [1], with confinement-induced resonances [1,2] allowing Feshbach resonance tuning [3] of the effective 1D interactions to very large values. This has led to experimental verification [4-6] of the fermionization of bosonic ultracold vapors in such geometries predicted by the Fermi-Bose (FB) mapping method [7], an exact mapping of a 1D gas of bosons with point hard-core repulsions, the "Tonks-Girardeau" (TG) gas, to an ideal spin-aligned Fermi gas. The "fermionic Tonks-Girardeau" (FTG) gas [8,9], a 1D spin-aligned Fermi gas with very strong attrac*tive* interactions, can be realized by a 3D *p*-wave Feshbach resonance as, e.g., in ultracold ⁴⁰K vapor [10]. It has been pointed out [2,8,9,11] that the FB mapping [7] can be exploited to map the FTG gas to the ideal Bose gas. The very strong fermion-fermion attraction in the FTG gas leads to fermion pairing and superconductive off-diagonal long-range order (ODLRO) of the two-fermion density matrix [12].

There are a number of models of strongly interacting 1D ultracold gas mixtures which are exactly solvable by generalizations of the FB mapping [13]. In [13,14] the properties of one such solvable model, a mixture of a TG Bose gas A and an ideal Fermi gas B, with point hard-core AB interactions, were investigated in detail. Here I shall discuss another model, a mixture of two different ideal Bose gases A and B, with an AB interaction of FTG form. This model is exactly solvable, and it will be shown that it has very unusual behavior: The strong AB attraction destroys the ground state Bose-Einstein condensation (BEC) and single-particle ODLRO of both components A and B, and it induces both AA and BB pairing manifested in superconductive ODLRO of the two-particle density matrices of components A and B, although there are no AA or BBinteractions. Furthermore, there is no AB pair ODLRO in spite of the strong AB attractions. It will also be shown that if the AB attraction is a finite odd-wave attraction rather PACS numbers: 67.85.-d, 03.75.Mn, 05.30.Jp

than the infinite FTG limit, and there is also a repulsive even-wave AB interaction of Lieb-Liniger (LL) delta function form [15], then there is a quantum phase transition as the coupling constants are varied, between a phase in which there are no AB contact nodes and only the repulsive LL interaction acts, and another phase in which there are AB contact nodes and only the attractive FTG-like interaction acts.

FTG interaction and nodal structure.—The FTG gas is a spin-aligned 1D Fermi gas with infinitely strongly attractive zero-range odd-wave interaction induced by a *p*-wave Feshbach resonance. It is the infinite 1D scattering length limit $a_{1D} \rightarrow -\infty$ of a 1D Fermi gas with zero-range attractive interactions leading to a 1D scattering length defined in terms of the ratio of the derivative Ψ' of the wave function to its value at contact: $\Psi(x_{ik} = 0+) = -\Psi(x_{ik} = 0+)$ $(0-) = -a_{1D}\Psi'(x_{jk} = 0\pm)$ where the prime denotes the derivative with respect to x_{ik} [2,8,9]. The FTG limit $a_{1D} \rightarrow$ $-\infty$ corresponds to a 1D zero-energy odd-wave scattering resonance reachable by Feshbach resonance tuning to a 1D odd-wave confinement-induced resonance [1-3]. There are several different zero-range pseudopotentials which generate this contact condition. One representation [8] is $\hat{v}_o = g_o \delta'(x_{jk}) \hat{\partial}_{\pm}$ where $\hat{\partial}_{\pm} \Psi(x_{jk}) = (1/2) \times$ $[\Psi'(0+) + \Psi'(0-)]$. The FTG limit $a_{1D} \rightarrow -\infty$ is equivalent to $g_{\rho} \rightarrow +\infty$. This representation explicitly exhibits an odd-wave projection property of the interaction; i.e., it vanishes on even functions of x_{ik} .

Since there is no particular symmetry under exchange of particles of the different species *A* and *B*, *AB* scattering in all partial waves is possible, but usually *s*-wave scattering dominates. However, in the neighborhood of a *p*-wave *AB* resonance, *p*-wave scattering dominates, and gives rise in 1D to an odd-wave effective interaction of FTG form [2,8,9]. For this it is important to realize that the odd-wave projection property of \hat{v}_o requires only *local* antisymmetry; i.e., it guarantees that if x_i is an *A*-particle position and y_i a *B*-particle position, then $\hat{v}_o \Psi(x_i, y_i)$ is

nonzero only if Ψ has a node at $x_i = y_j$, where $\Psi(x_i, y_j) = -\Psi(y_j, x_i)$ in an *infinitesimal* neighborhood of the node. It is not necessary that there be *global* antisymmetry under such exchange, and indeed, the ground state Ψ_0 derived in the following sections has no such global antisymmetry. In the presence of both a 1D even-wave *AB* Lieb-Liniger interaction $g_e \delta(x_i - y_j)$ [15] generated by 3D *s*-wave *AB* scattering and a 1D odd-wave resonance generated by a 3D *p*-wave Feshbach resonance for *AB* scattering, the wave function can lower its energy by developing nodes at $x_i = y_j$ so as to kill the repulsive even-wave interaction and activate the strong 1D odd-wave attraction.

The contact discontinuities of Ψ [11] can also be understood as a zero-range limit $x_0 \to 0+$ and $V_0 \to \infty$ of the two-body scattering solution for a square well of width $2x_0$ and depth V_0 , where the limit is carried out such that $V_0 x_0^2$ approaches a finite, nonzero limit [8,9]. In the untrapped case, the exterior solution for scattering length $a_{AB} \to -\infty$ is constant (+1 for x - y > 0 and -1 for x - y < 0), and the interior solution is $\sin[\kappa(x - y)]$ with $\kappa = \sqrt{2\mu V_0/\hbar^2} = \pi/2x_0$ and μ the effective mass $m_A m_B/(m_A + m_B)$; hence, $\kappa x_0 = \pi/2$ and $V_0 x_0^2 = (\pi\hbar)^2/8\mu$. In the zero-range limit the interior kinetic energy $\to +\infty$ and potential energy $\to -\infty$, but their sum remains zero, the ground state energy. Since the FTG interaction acts only on odd waves, the FTG interaction \hat{v}_0 should be written as $\hat{v}_0 = v(x)\hat{P}_0$ where v(x) is the above square well and \hat{P}_0 is the odd-wave projector.

Many-body ground state.—Assuming trapping on a ring, the Hamiltonian consists only of the kinetic energy operators of components *A* and *B* plus the *AB* FTG interaction:

$$\hat{H} = \sum_{i=1}^{N_A} \frac{-\hbar^2}{2m_A} \frac{\partial^2}{\partial x_i^2} + \sum_{i=1}^{N_B} \frac{-\hbar^2}{2m_B} \frac{\partial^2}{\partial y_i^2} + \sum_{i=1}^{N_A} \sum_{j=1}^{N_B} \hat{v}_o(x_i - y_j),$$
(1)

where \hat{v}_{o} is the previously defined odd-wave FTG interaction. The wave functions satisfy periodic boundary conditions with periodicity length L (the ring circumference) with respect to all the x_i and y_i . The scattering length a_{AB} is $-\infty$ in the FTG limit. For square well width $2x_0$ nonzero but very small, the unnormalized ground state Ψ_0 is constant (say ± 1) when all $|x_i - y_j| > 2x_0$, except for sign changes as each $x_i - y_i$ varies from $-x_0$ to x_0 in accordance with the internal wave function $\pm \sin[\kappa(x_i - y_i)]$. The condition $\kappa = \sqrt{2\mu V_0/\hbar^2} = \pi/2x_0$ determines the well depth V_0 such that the scattering length a_{AB} is $-\infty$, and the FTG limit is obtained by letting $x_0 \rightarrow 0$ and $V_0 \rightarrow 0$ ∞ in accordance with this condition. In this limit the internal wave function becomes invisible and Ψ_0 appears to jump discontinuously between ± 1 whenever an A particle passes a *B* particle, but there are hidden nodes at x_i – $y_i = 0$ at the centers of the wells. The ground state energy $E_0 = 0$, generalizing the situation for the pure FTG gas [2,8,9,12]. Ψ_0 maps to a "model state" Ψ_{M0} consisting of two noninteracting ideal Bose gases totally Bose-Einstein condensed into their ground orbital, which is a trivial constant for periodic boundary conditions: $\Psi_0 =$ $\Psi_{M0}M = M$ and $\Psi_{M0} = 1$ where *M* is the mapping function

$$M(x_1, \dots, x_{N_A}; y_1, \dots, y_{N_B}) = \prod_{i=1}^{N_A} \prod_{j=1}^{N_B} \operatorname{sgn}(x_i - y_j), \quad (2)$$

where the sign function sgn(x) is +1(-1) if x > 0 (x < 0). Although the mapped bosonic state Ψ_{M0} is a trivial constant outside the square wells, the interior wave function $\pm \sin(\kappa |x_i - y_j|)$ vanishes with cusps at $x_i - y_j = 0$. Therefore, physical consistency requires the presence of a zero-diameter hard-core interaction added to the square well. The mapped Bose gas is then not truly ideal, but rather a TG gas with superimposed attractive well, whose nontrivial interior wave function becomes invisible in the zero-range limit, simulating a mixture of two noninteracting ideal Bose gases insofar as the energy and exterior wave function are concerned. The densities of components A and B are trivial constants in the ground state, but the offdiagonal elements of the reduced density matrices of Ψ_0 are quite nontrivial and interesting, due to the effects of the discontinuities in M; they will be discussed in later sections.

The periodic boundary conditions impose constraints on the values of N_A and N_B . Suppose that the positions of all *B* bosons and all but one *A* boson, say x_1 , are fixed on the open interval (0, *L*). Starting with that *A* boson at $x_1 > 0$ but to the left of all the other particles and moving it to a position $x_1 < L$ but to the right of all the others, one counts N_B sign changes of Ψ_0 due to the *AB* contact nodes, so N_B must be even for *L* periodicity in the *A*-boson coordinates. Repeating this process with all *A* bosons and all but one *B* boson fixed and moving that *B* boson instead, one counts N_A sign changes; hence, N_A must be even for *L* periodicity in the *B*-boson coordinates.

One-particle density matrices and momentum distributions.—Generalizing the derivation in [12,16,17], one finds that the one-particle density matrix of component A is

$$\rho_{1A}(x, x') = N_A L^{-N_A - N_B} \int \Psi_0(x, x_2, \dots, x_{N_A}; Y) \times \Psi_0(x', x_2, \dots, x_{N_A}; Y) dx_2 \cdots dx_{N_A} dY = n_A [I(x, x')]^{N_B},$$
(3)

where $Y = (y_1, ..., y_{N_B})$, $n_A = N_A/L$, and $I(x, x') = L^{-1} \int_{-L/2}^{L/2} \operatorname{sgn}(x - \xi) \operatorname{sgn}(x' - \xi) d\xi = 1 - 2|x - x'|/L$. In the thermodynamic limit where $N_B \to \infty$ and $L \to \infty$ such that $N_B/L \to n_B$ with finite and nonzero number density n_B , one has $[I(x, x')]^{N_B} \to e^{-2n_B|x-x'|}$ in analogy with the one-component FTG gas case [12,16,17]. Hence, $\rho_{1A}(x, x') = n_A e^{-2n_B|x-x'|}$, and by interchange of A and B $\rho_{1B}(y, y') = n_B e^{-2n_A|x-x'|}$. Their Fourier transforms n_{kA} and n_{kB} , normalized to $\sum_k n_{kA} = N_A$ and $\sum_k n_{kB} = N_B$ where the allowed momenta are $k = \nu 2\pi/L$ with $\nu = 0, \pm 1, \pm 2, ...$), are Lorentzian discrete momentum distributions $n_{kA} = \frac{4n_A n_B}{4n_B^2 + k^2}$ and $n_{kB} = \frac{4n_A n_B}{4n_A^2 + k^2}$. The Fermi-like Lorentzian shapes are strong modifications of the ideal Bose gas distributions $N_A \delta_{k0}$ and $N_B \delta_{k0}$ due to the infinite AB attraction; no trace of BEC of components A and B, and of the associated ODLRO of ρ_{1A} and ρ_{1B} , remains. Nevertheless, at k = 0, n_{kA} reduces to n_A/n_B which increases without limit as the *B*-component density n_B falls to zero for fixed n_A , and in fact the continuous momentum distribution $(L/2\pi)n_{kA}$ reduces to a representation of the ideal Bose gas distribution $N_A\delta(k)$ as $n_B \rightarrow 0$. n_{kB} has the same behavior, with *A* and *B* interchanged.

Two-particle density matrices, pairing, and ODLRO.— The two-particle *A*-component and *B*-component density matrices $\rho_{2AA}(x_1, x_2; x'_1, x'_2)$ and $\rho_{2BB}(y_1, y_2; y'_1, y'_2)$ can also be evaluated in closed form by generalization of (3) and the derivation for the one-component FTG gas in [12]. For component *A*

$$\rho_{2AA}(x_1, x_2; x_1', x_2') = N_A(N_A - 1)L^{-(N_A + N_B)} \int \Psi_0(x_1, x_2, x_3, \dots, x_{N_A}; Y)\Psi_0(x_1', x_2', x_3, \dots, x_{N_A}; Y)dx_3 \cdots dx_{N_A} dY.$$
(4)

Using $\Psi_0(x_1, x_2, x_3, \dots, x_{N_A}; Y) = \prod_{j=1}^{N_B} \operatorname{sgn}(x_1 - y_j) \operatorname{sgn}(x_2 - y_j)$ one finds in the thermodynamic limit $\rho_{2AA}(x_1, x_2; x_1', x_2') = n_A^2 e^{2n_B(z_1 - z_2 + z_3 - z_4)}$, where $z_1 \le z_2 \le$ $z_3 \le z_4$ are the arguments $(x_1, x_2; x'_1, x'_2)$ in ascending order. If $x_1 < x_2 < x'_1 < x'_2$, then $\rho_{2AA} = n_A^2 e^{-2n_B |x_1 - x_2|} e^{-2n_B |x'_1 - x'_2|}$. Generalizing the argument in [12] one sees that if the variable pairs (x_1, x_2) and (x'_1, x'_2) are separated to arbitrary distance while keeping $|x_1 - x_2|$ and $|x_1' - x_2'|$ fixed, then ρ_{2AA} remains constant, signaling AA-pair ODLRO associated with a leading term $\lambda_{1AA}u_{1A}(x_1, x_2)u_{1A}(x_1', x_2')$ in the spectral representation of ρ_{2AA} , with eigenfunction $u_{1A}(x_1, x_2) = C_A e^{-2n_B|x_1-x_2|}$, normalization constant $C_A = \sqrt{2n_B/L}$, and macroscopic eigenvalue $\lambda_{1AA} = n_A^2/C_A^2 = n_A N_A/2n_B$. There is a BEC-BCS crossover from AA-pair BEC when $n_B \gg n_A$ and the range of u_{1A} is $\ll 1/n_A$, implying tightly bound AA pairs, to AA-pair superconductivity when $n_B \ll n_A$ and the range of u_{1A} is $\gg 1/n_A$, implying extended and strongly overlapping AA Cooper pairs. Since $\rho_{2BB}(y_1, y_2; y'_1, y'_2)$ exhibits the same behavior with A and B interchanged, one concludes that when $n_B \gg n_A$ there is coexistence of BEC of AA pairs and superconductivity of BB pairs, and when $n_B \ll n_A$ there is coexistence of BEC of BB pairs and superconductivity of AA pairs. The AA and BB pairing is a purely off-diagonal phenomenon, both in the case of superconductive ODLRO with weakly bound Cooper pairs and in the case of BEC of tightly bound pairs. There is no diagonal AA, BB, or AB order; the pair distribution functions $D_{AA}(x_1, x_2) = n_A^{-2} \rho_{2AA}(x_1, x_2; x_1, x_2),$ $D_{BB}(y_1, y_2) = n_B^{-2} \rho_{2BB}(y_1, y_2; y_1, y_2), \text{ and } D_{AB}(x, y) =$ $(n_A n_B)^{-1} \rho_{2AB}(x, y; x, y)$ are all constant, as is most easily seen by noting that (a) our system of A bosons and Bbosons with FTG AB attraction maps to a mixture of ideal A-Bose and B-Bose gases with no AB interaction, and (b) diagonal density matrix elements are invariant under mapping via Eq. (2). This generalizes the previous result for the pure FTG gas, where there is superconductive ODLRO but the pair distribution function is constant [12].

The two-particle AB density matrix is also of interest. By a derivation paralleling that for ρ_{2AA} and ρ_{2BB} one finds in the thermodynamic limit

$$\rho_{2AB}(x, y; x', y') = n_A n_B \operatorname{sgn}(x - y) \operatorname{sgn}(x' - y') \\ \times e^{-2n_B |x - x'|} e^{-2n_A |y - y'|}.$$
(5)

Suppose that x' = x + d and y' = y + d. Then $\rho_{2AB} =$ $n_A n_B e^{-2(n_A + n_B)d}$ which vanishes exponentially as $d \to \infty$. It follows that there is no AB-pair ODLRO in spite of the strong AB attraction. It is informative in this connection to compare and contrast two cases (a) two ideal Bose gases A and B with no AB interactions, and (b) the present case, two ideal Bose gases A and B with FTG AB interactions. In case (a) there is complete BEC of both components A and B, the many-body ground state is a trivial constant, ρ_{2AA} , ρ_{2BB} , and ρ_{2AB} are also constant, and hence all three of these density matrices exhibit ODLRO. However, the AA and BB ODLRO is a trivial consequence of the trivial ground state structure and, more generally, follows from the ODLRO of ρ_{1A} and ρ_{1B} [18] and implies no true AA or BB pairing correlation. In the present case (b), there is no BEC of component A or B and hence no ODLRO of ρ_{1A} or ρ_{1B} , but there is ODLRO of both ρ_{2AA} and ρ_{2BB} , implying both AA and BB pairing, since u_{1A} and u_{1B} have finite range. On the other hand, ρ_{2AB} has no ODLRO.

Quantum phase transition.-Suppose now that in addition to the odd-wave AB interaction of FTG form, there is also an even-wave AB interaction of LL delta function form [15], $v_e(x_i - y_i) = g_{AB}\delta(x_i - y_i)$ with $g_{AB} > 0$ (repulsive interaction). Recall that before passing to the infinitely narrow well limit $x_0 \rightarrow 0$, $V_0 \rightarrow \infty$ of the FTG interaction, the ground state in the case of no even-wave interaction has nodes at AB contact due to the internal wave function $\sin \kappa (x_i - y_i)$. These nodes kill the evenwave interaction, so that the ground state in the presence of the even-wave interaction is the same as that in the absence of an even-wave interaction, which has energy zero. Any state without AB contact nodes has positive energy in the presence of the even-wave repulsion, since then the oddwave FTG interaction is killed; the system develops ABcontact nodes spontaneously in the presence of the FTG

odd-wave attraction in order to lower its energy by killing the even-wave repulsion. Now suppose that there is no even-wave interaction, but the odd-wave attraction is weakened by carrying out the limit $x_0 \rightarrow 0$ and $V_0 \rightarrow \infty$ in such a way as to produce a large but finite negative oddwave scattering length, $-\infty < a_{ABo} < 0$. So far the FTG limit where $\kappa x_0 = \frac{\pi}{2}$ and $a_{ABo} = -\infty$ has been assumed, but more generally if a_{ABo} is negative and finite, then $\kappa x_0 = \frac{\pi}{2} - \frac{2x_0}{\pi |a_{ABo}|}$ as $x_0 \to 0$ [9,19]. The ground state Ψ_0 in that case maps via (2) to a model ground state Ψ_{M0} consisting of two Bose gases A and B with no AA or BB interaction but an even-wave AB interaction of LL form $g'_{AB}\delta(x_i - y_i)$ with $g'_{AB} = \hbar^2/\mu |a_{ABo}|$ and positive energy. If one generalizes further by adding a nonzero even-wave interaction $g_{AB}\delta(x_i - y_i)$ again, then so long as the ground state Ψ_0 is retained unchanged with AB contact nodes, the even-wave interaction will be killed and will have no effect. However, if $g_{AB} < g'_{AB} = \hbar^2/\mu |a_{ABo}|$, then a ground state with no *AB* contact nodes has lower energy, since then it is the odd-wave interaction which is killed, instead of the even-wave interaction. It follows that there is a quantum phase transition between a phase with no ABcontact nodes, which has lower energy when $g_{AB} < g'_{AB}$, and a phase with AB contact nodes, which has lower energy when $g_{AB} > g'_{AB}$. This is very similar to the ferromagneticantiferromagnetic phase transition in the 1D spinor Fermi gas with both even- and odd-wave interactions [20,21].

Stronger AB attraction.-It was pointed out above that if $-\infty < a_{ABo} < 0$ then $\kappa x_0 = \frac{\pi}{2} - \frac{2x_0}{\pi |a_{ABo}|}$ as $x_0 \rightarrow 0$, or with-out the absolute value signs $\kappa x_0 = \frac{\pi}{2} + \frac{2x_0}{\pi a_{ABo}}$. In analogy with the case of fermions discussed recently [22], for an interaction of FTG form the same relation (without absolute value signs) holds if $a_{ABo} > 0$, in which case the model state Ψ_{M0} generated by the mapping (2) has an *attractive* LL AB interaction $g_{AB}\delta(x_i - y_j)$ with $g_{AB} =$ $-\hbar^2/\mu a_{ABo} < 0$ and *negative* energy. The N = 2 model ground state is bound, $\Psi_{0M} = e^{-|x-y|/a_{ABo}}$ with energy $E_0 = -\frac{\hbar^2}{2\mu a_{ABo}^2}$, and the corresponding actual physical state is $\Psi_0 = \operatorname{sgn}(x - y)e^{-|x-y|/a_{ABo}}$, with the same energy. The exact solution for both $N_A > 2$ and $N_B > 2$ is not known, but if Ψ_{M0} has Bijl-Jastrow form $\Psi_{M0} =$ $\mathfrak{N}\prod_{i=1}^{N_A}\prod_{j=1}^{N_B}f(|x_i - y_j|)$ where \mathfrak{N} is a normalization constant and $f(|x_i - y_j|) \approx e^{-|x_i - y_j|/a_{ABo}}$ for $|x_i - y_j| \ll$ $(\sqrt{n_A n_B})^{-1}$, then in the neighborhood of each $x_i - y_i =$ 0 the wave function reduces to that of an AB dimer. The behavior of Ψ_{M0} as x_i recedes to distances $x_i \gg$ $(\sqrt{n_A n_B})^{-1}$ from y_i will be controlled by proximity of x_i to other *B* particles, not y_i . If $f(\xi) \to \lambda$ for $\xi \gg$ $(\sqrt{n_A n_B})^{-1}$ where λ is some nonzero constant, then $\Re =$ λ^{-N_B} . The physical state Ψ_0 generated by the mapping (2) then has reduced density matrices reducible to 1D integrals as previously. However, in the thermodynamic limit ρ_{2AB} reduces to the previous expression (5), with no *AB*-pair ODLRO. A better approximation to Ψ_0 might reverse this conclusion, so this model deserves further study.

Outlook.—In view of the surprising properties of this model, experimental study of mixtures of weakly interacting *A* bosons and *B* bosons in tight waveguides with strong 1D *AB* attractions [2] induced by a *p*-wave *AB* Feshbach resonance [10] should be fruitful. In particular, one could look for the predicted quantum phase transition.

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