Inhomogeneous State of Few-Fermion Superfluids

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The few-fermion atomic gas is an ideal setting to explore inhomogeneous superfluid pairing analogous to the Larkin-Ovchinnikov state. Two up and one down-spin atom is the minimal configuration that displays an inhomogeneous pairing density, whereas imbalanced systems containing more fermions present a more complex pairing topology. With more than eight atoms trapped the system approaches the macroscopic superfluid limit. An oblate trap with a central barrier offers a direct experimental probe of pairing inhomogeneity.

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The rapidly advancing field of ultracold atomic gases has opened new vistas of experimentally accessible phases of matter. The observation of superfluidity [1–4] and density imbalance [5,6] in a two-component Fermi gas presents the building blocks required to realize the inhomogeneous superfluid phase proposed by Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) [7,8]. This state plays a central role in our understanding of superconductors, superfluids, and particle physics [9] but has never been unambiguously realized in solid state superconductors [10]. Theory predicts that the FFLO phase should be present in a three-dimensional atomic gas; however, it has not been observed [5,6]. In a one-dimensional imbalanced atomic gas, although the superfluid is predicted to be stable [11,12], any inhomogeneous pairing present was too weak to be observed [13,14]. We now exploit the new experimental capability to trap, manipulate, and address a few fermionic atoms [15,16] to propose a protocol to create an inhomogeneous superfluid. The pairing has a simple nodal structure that can be directly characterized by experiment.

To study the few-fermion superfluid we take advantage of recent experimental developments that allow investigators to confine up to ten atoms in a trap and address their quantum state [15–17]. This presents a unique opportunity to study the microscopic physics of contact interactions [18–25] in a tractable setting, and then scale the intuition up to a many-body system. Following this program, experimentalists could realize an analog to the Stoner model for itinerant ferromagnetism [26,27], and the direct and double exchange mechanisms [28]. We now turn from repulsive to attractive interactions to study a counterpart to the BCS superconductor. Though the three-fermion ground state has been previously examined [29,30] in both three and one dimension [31], the authors overlooked the underlying inhomogeneous pairing.

To orient the discussion we first expose the symmetry changes in the ground state that foretell the emergence of inhomogeneous pairing. Next we study the inhomogeneous pairing for a state with $N_\uparrow$ up-spin atoms and $N_\downarrow$ down-spin atoms, showing that the number of nodes in the pairing density is $N_\uparrow - N_\downarrow$. Therefore, to render a straightforward pairing topology we focus on the few-fermion system. The simple spatial distribution couples to the trap oblateness and a central barrier allowing us to propose a direct experimental probe of the pairing inhomogeneity. The two up and one down-spin excited states are prototypes for the ground state of many-body systems. Moreover, with more than eight atoms trapped the system approaches the macroscopic superfluid state, motivating our program to probe the infinite-body system from a few-atom standpoint.

Formalism.—A fermionic gas of two hyperfine states is tightly confined to realize the Hamiltonian $\hat{H} = -\hbar^2\nabla^2/2m + m\omega_\perp^2(x^2+y^2)/2 + m\omega_\parallel^2 z^2/2 + g(\mathbf{r}_1 - \mathbf{r}_2)$, with m the atomic mass, and a harmonic oscillator length $a_\parallel = \sqrt{\hbar/m\omega_\parallel}$. We parametrize the interspecies potential $g(\mathbf{r}) = -U\Theta(R - |\mathbf{r}|)$ through an s-wave scattering length $a = R[1 - \tan(R\sqrt{mU}/\hbar)\hbar/R\sqrt{mU}]$. We denote the general state $|N_\uparrow, N_\downarrow\rangle$, and the (excited) state with symmetry $\alpha \in \{s, p, d, f, g\}$ as $|N_\uparrow, N_\downarrow\rangle^\alpha$.

Our main tool to study the ground and excited states is exact diagonalization. We use the Gaussian orbitals of the trapping potential $\phi_{n_x n_y n_z}(x, y, z)$ as the one-particle basis functions for the calculation, retaining all orbitals that satisfy $(n_x, n_y, n_z) \leq 5$. The matrix elements of the interaction in this basis set are evaluated numerically. We construct the $(N_\uparrow, N_\downarrow)$ Slater determinants in this basis set and retain the 10000 determinants with lowest non-interacting energy to form a many-body basis set in which to construct the Hamiltonian matrix. We diagonalize the matrix to obtain the energy eigenstates $\{\psi_m(a)\}$. We can connect the eigenstates at neighboring values of the scattering length a_i and a_{i+1} with maximal overlap $\langle\psi_m(a_i)|\psi_n(a_{i+1})\rangle$ to build up the band structure.

Ground state energy.—We first study the ground state energy and symmetry of the atoms in a spherical trap with $\omega_\perp = \omega_\parallel$. We start from the simplest interacting system $|1, 1\rangle$. At weak interactions both atoms occupy the ϕ_{000}

orbital so that the ground state is spherically symmetric. With increasing interactions the atoms adiabatically evolve into a tightly bound molecule that retains the same spherical symmetry. The bound fermionic atoms can now be regarded as a bosonic particle, but to expose this change in the underlying particle statistics we must introduce a second up-spin atom.

In the weakly interacting $|2,1\rangle$ system the new up-spin atom is forced by Pauli exclusion to enter one of the triply degenerate (ϕ_{100}, ϕ_{010}, ϕ_{001}) orbitals possessing p-wave symmetry. The next excited state shown in Fig. 1(a) places that atom into a singly degenerate superposition of the (ϕ_{200}, ϕ_{020}, ϕ_{002}) orbitals which will have s-wave symmetry. Above this there is a ninefold degenerate g-wave state (the ground p-wave state excited with center-of-mass motion so that it has triple the degeneracy of the p-wave state), then a fivefold degenerate d-wave state with zero center-of-mass motion, and above that many other disconnected excited states. Previous analysis of this system was performed in the center-of-mass frame so neglected the g-wave state [29,30]. On entering the strongly attractive regime an up and down-spin atom bind into a bosonic molecule, removing the Pauli blocking, leaving the excess up-spin atom in the ϕ_{000} orbital. There must be a crossing from the weakly interacting p-wave to the strongly interacting s-wave regime. In Fig. 1(b) we plot the energy difference between the ground and first excited states. This shows that the transition from p to s-wave symmetry occurs at $a = 0.46a_{\|}$, a crossing phenomenon similar to that suggested in Refs. [29–31]. In general the up and down-spin atoms bind in pairs, leaving any excess majority spins to fill orbitals as if they were noninteracting, and adopting the symmetry of that state. This can lead to a changing symmetry of the ground state that betrays the innate inhomogeneous pairing.

Having seen the consequences of the ground state symmetry changing with the introduction of the extra up-spin atom we now introduce a further up-spin atom giving $|3,1\rangle$. The weakly interacting ground state carries p-wave symmetry that adiabatically connects with the strongly interacting ground state where the two excess up-spin atoms also have p-wave symmetry. Therefore Fig. 1(b) shows that this triply degenerate state is always lower in energy than the next family of excited states so the system should display inhomogeneous pairing at all interaction strengths. We next examine the $|4,1\rangle$ system. In the weakly interacting regime the majority spins occupy a full shell of (ϕ_{100}, ϕ_{010}, ϕ_{001}) orbitals so the ground state has s-wave symmetry. In the strongly interacting regime one of the up-spin atoms is bound to the down spin at $a = 0.31a_{\|}$, fragmenting the full shell into a p-wave ground state. Finally, we verify that the $|2,2\rangle$ system has a spherically symmetric ground state at all interaction strengths indicating that this balanced system will not display inhomogeneous pairing. The first excited states display d-wave symmetry. Although they are degenerate with the ground state in the noninteracting limit, the energy difference grows rapidly with rising interactions. When the energy difference exceeds $\hbar\omega_{\|}$ a p-wave state (the s-wave state excited with center-of-mass motion) becomes the new lowest excited state. This crossing produces the kink at $a \approx 1.2a_{\|}$.

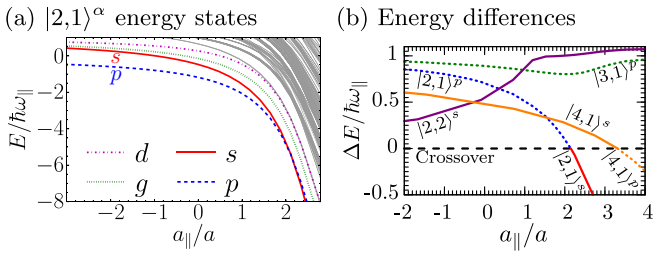

FIG. 1 (color online). (a) The energy bands of the $|2,1\rangle$ system, highlighting the p-wave state (blue dashed), s-wave state (red solid), g-wave (green dots), d-wave (magenta dot-dashed), and higher excited states in gray. (b) The difference in energy between the two lowest eigenstates with increasing number of atoms. Solid lines denote an s-wave ground state and dashed a p-wave ground state. Different colors denote the labeled states, with the same colors depicting the $|2,1\rangle$ state in both (a) and (b). The horizontal black dashed line delineates the crossover between the two lowest eigenstates.

Inhomogeneous pairing.—In the presence of a population imbalance the ground state symmetry can switch with interaction strength, raising the possibility of inhomogeneous pairing. This motivates us to study the underlying pairing density. We measure the pairing correlations with the expectation value $\bar{\Delta}(\mathbf{r})\Delta(\mathbf{0}) = \langle c_{\uparrow}^{\dagger}(\mathbf{r})c_{\downarrow}^{\dagger}(\mathbf{r})c_{\downarrow}(\mathbf{0})c_{\uparrow}(\mathbf{0})\rangle$ that explicitly conserves the number of atoms. In Fig. 2 we compare the isosurfaces of equal spin imbalance $\langle c_{\uparrow}^{\dagger}c_{\uparrow} - c_{\downarrow}^{\dagger}c_{\downarrow}\rangle$ with the interaction strength independent isosurface of equal pairing growth rate, $d(\bar{\Delta}\Delta)/da|_{a=0}$.

We start with $|2,1\rangle$ atoms, the minimal system that exhibits an inhomogeneous ground state. Without loss of generality we place the upper majority spin atom into the ϕ_{001} orbital, fixing the excess density along the z axis as shown in Fig. 2(a). Within first order perturbation theory the ground state $c_{000\uparrow}^{\dagger}c_{001\uparrow}^{\dagger}c_{000\downarrow}^{\dagger}|0\rangle$ couples to the transverse states $c_{100\uparrow}^{\dagger}c_{001\uparrow}^{\dagger}c_{100\downarrow}^{\dagger}|0\rangle$ and $c_{010\uparrow}^{\dagger}c_{001\uparrow}^{\dagger}c_{010\downarrow}^{\dagger}|0\rangle$. The induced pairing is inhomogeneous as Pauli blocking prevents the atoms from coupling to $c_{001\uparrow}^{\dagger}c_{001\uparrow}^{\dagger}c_{001\downarrow}^{\dagger}|0\rangle$. The pairing correlations $\bar{\Delta}(\mathbf{r})\Delta(\mathbf{0}) \propto (x^2 + y^2)\exp(-\omega_{\|}r^2)$ and excess spin density $\sim z^2\exp(-\omega_{\|}r^2)$ yield the isosurfaces shown in Fig. 2(a). The pairing is peaked in the regions of low excess up-spin atom density. This distribution is similar to that proposed for the low-density one-dimensional FFLO state [32,33]. We can probe the emergence of inhomogeneous pairing correlations by studying the spherical harmonics present in the pairing function in Fig. 2(g). The $\ell = 2$ component grows rapidly with interaction strength signifying the pairing increasing only within the

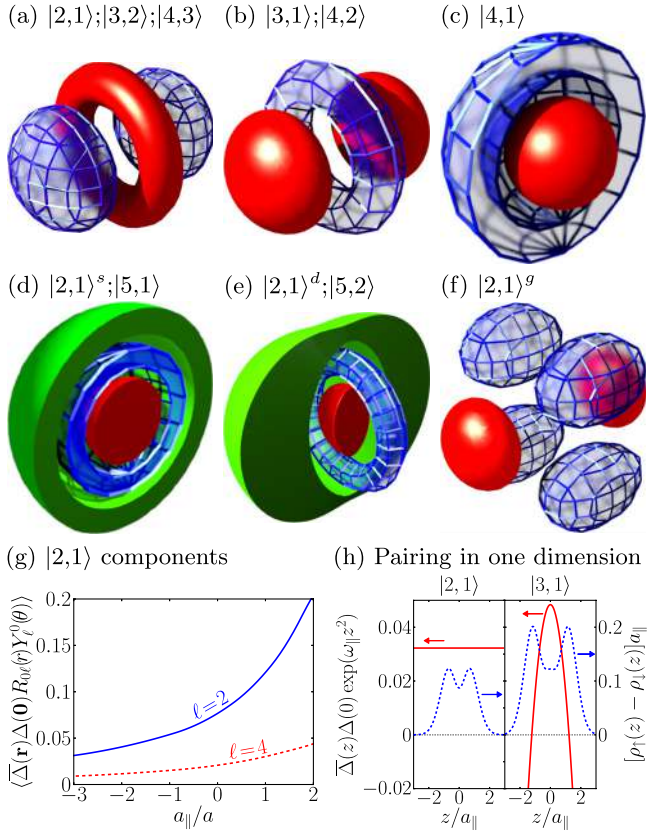

FIG. 2 (color online). (a)–(f) The isosurfaces of the pairing density (positive: red; negative: green), and excess majority spin density (blue mesh). (g) the angular spherical harmonic components of the $|2,1\rangle$ system where $R_{n\ell}$ are the radial solutions for principal quantum number n and orbital quantum number ℓ, and Y_ℓ^m denotes the spherical harmonic function with projected angular momentum quantum number m. (h) shows the pairing density (red solid) and excess spin density (blue dashed) in a one-dimensional system.

torus, and the $\ell = 4$ component increases so that the pairing can rise abruptly at the boundary between torus and the excess majority spin density. The excess majority spin mostly remains in the ϕ_{001} orbital.

Now that we have studied the inhomogeneous pairing of the $|2,1\rangle$ ground state we turn to reexamine the excited states from Fig. 1(a). These are not only accessible through radio frequency transfers, but, moreover, act as precursors of states containing more atoms so will help develop our intuition. We enumerate the three lowest excited states in Figs. 2(d)–2(f) that all exhibit inhomogeneous pairing. The $|2,1\rangle^s$ state in Fig. 2(d) is formed by taking the up-spin atom from the ϕ_{001} orbital and exciting it into the spherically symmetric linear combination of the $(\phi_{200},\phi_{020},\phi_{002})$ orbitals. The majority spin atom lies in a shell at the node of the pairing density. The $|2,1\rangle^d$ state in Fig. 2(e) is formed by exciting an atom out of the ϕ_{000} orbital and into the $(\phi_{200}+\phi_{020})/2-\phi_{002}$ orbital. The excess spin now lies in a torus that defines the pairing node. The $|2,1\rangle^g$ state Fig. 2(f) is formed by exciting $|2,1\rangle$ with center-of-mass motion in the x-y plane, thereby breaking the cylindrical symmetry. These excited states contain low energy vacant orbitals (e.g., ϕ_{000}) into which we can insert further atoms to form new ground states.

With our study of the minimal $|2,1\rangle$ system complete we now study systems containing more atoms. First, we examine the $|3,1\rangle$ system. Figure 2(b) reveals that the majority spins lie in the x-y plane focusing the pairing along the z axis. The $|4,1\rangle$ system has a full $n=1$ shell of excess spin atoms. The pairing density is spherically symmetric, enveloped by the excess spin density. The conformation of the nodal surface is commensurate with the number of excess fermions. To verify this conjecture we first look at the $|3,2\rangle$ and $|4,3\rangle$ systems. Although the occupied orbitals contrast to the $|2,1\rangle$ system, each has one excess spin fermion with an identical pairing structure. Likewise the $|4,2\rangle$ system has an identical topology to the $|3,1\rangle$. The $|3,1\rangle$; $|4,2\rangle$; $|4,1\rangle$ states have no counterpart in the spectrum of the $|2,1\rangle$ excitations because they rely on the occupation of the (ϕ_{100},ϕ_{010}) orbitals that do not couple to the $|2,1\rangle$ state so to connect with the excited states we now turn to systems containing more atoms.

In the $|5,1\rangle$ system Fig. 2(d) the new atoms first fill the (ϕ_{100},ϕ_{010}) orbitals and then the final new atom enters a linear combination of the $(\phi_{200},\phi_{020},\phi_{002})$ orbitals, rendering a spherically symmetric state. This can be regarded as the $|2,1\rangle^s$ state but with the $(\phi_{100},\phi_{010},\phi_{001})$ orbitals filled and so adopts the same topology. Likewise, the $|5,2\rangle$ system can be regarded as the $|2,1\rangle^d$ state with the $(\phi_{000},\phi_{100},\phi_{010},\phi_{001})$ orbitals filled. This state with three excess fermions notably has a different topology to the $|4,1\rangle$ state with equal imbalance due to the newly occupied $n=2$ shell having greater degeneracy with atoms entering the ϕ_{110} orbitals that induce d-wave character. The ability to build many-particle states out of the excited states of a few-atom system illustrates the utility of studying the few-atom systems to understand many-body states. In Fig. 3(b) we connect to the macroscopic FFLO state by studying

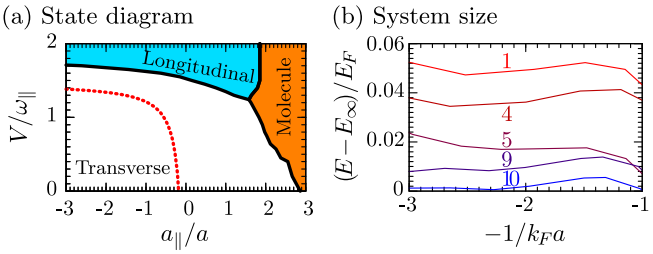

FIG. 3 (color online). (a) The ground state for two up and one down-spin atom in the trap $\omega_\perp = 0.5\omega_\parallel$ with changing barrier height V and interaction strength a. The blue shaded region denotes the longitudinal ground state, the white area the transverse state, and orange the molecular state. The red dashed line denotes the longitudinal-transverse boundary predicted by perturbation theory. (b) The energy of a single down spin embedded in N up-spin atoms compared with the infinite system size limit, with k_F defined from the noninteracting Fermi energy.

how the energy varies with system size, and compare to the 3D polaron limit that can be solved analytically [34]. With more than eight atoms trapped the energy approaches the infinite-body polaron limit, showing that the few-atom system directly links to the macroscopic state.

Finally, we examine the pairing in a one-dimensional system with $\omega_\perp = 10\omega_\parallel$. Starting again with $|2,1\rangle$ the pairing is concentrated at the center, forcing the excess majority atom outwards. This configuration is analogous to the $|2,1\rangle$ in the spherical trap that we studied earlier, projected onto the z axis. With further atoms present, such as $|3,1\rangle$ each excess up-spin atom sits at $z \approx \pm\sqrt{3/2}a_\parallel$, with the pairing changing sign as it crosses through a node at these points. This confirms our picture of the majority spin atom defining nodes in the pairing correlations, similar to that proposed for the low-density FFLO state [32,33]. Though this one-dimensional system is realizable, the spatial inhomogeneity would be difficult to probe in experiment. Instead, we now return to the three-dimensional system and exploit the state degeneracy to propose an experimental observable.

Experimental observation.—Following the emergence of inhomogeneous pairing we now take advantage of the simple spatial variation of the pairing in the $|2,1\rangle$ FFLO state to propose an experimental observable. Two parameters couple to the angular pairing oscillations: a pancake trapping potential with $\omega_\parallel > \omega_\perp$ encourages the unpaired majority spin atom into a doubly degenerate transverse orbital (ϕ_{100} or ϕ_{010}), whereas a central barrier $V\exp(-\omega_B z^2)$ favors occupation of the singly degenerate longitudinal orbital (ϕ_{001}) that has a node over the barrier. Strong inhomogeneous pairing attracts density towards the energetically costly central barrier so to minimize that density the system favors the occupation of the longitudinal state. This transition provides a direct probe of the inhomogeneous pairing.

We use both exact diagonalization and first order perturbation theory to probe the boundary between the transverse and longitudinal states. Starting from the noninteracting states in the absence of the central barrier we include both the interactions and the barrier through first order perturbation theory to yield the estimates for the ground state energy

$$\begin{aligned}\text{Longitudinal, singly degenerate}\quad & \frac{5}{2}\omega_\parallel + 3\omega_\perp + V\sqrt{\frac{\omega_\parallel}{\omega_\parallel+\omega_B}}\left(2+\frac{\omega_\parallel}{\omega_\parallel+\omega_B}\right) + \frac{a}{a_\parallel}\omega_\perp\sqrt{\frac{2}{\pi}}\left(\frac{3}{2}-\frac{4\sqrt{2}}{\pi}\frac{V}{\omega_\parallel+\omega_B}\right)\\ \text{Transverse, doubly degenerate}\quad & \frac{3}{2}\omega_\parallel + 4\omega_\perp + 3V\sqrt{\frac{\omega_\parallel}{\omega_\parallel+\omega_B}} + \frac{a}{a_\parallel}\omega_\perp\sqrt{\frac{2}{\pi}}\left(\frac{3}{2}-\frac{6\sqrt{2}}{\pi}\frac{V}{\omega_\parallel+\omega_B}\right).\end{aligned} \tag{1}$$

Setting the two energies equal predicts a crossover at

$$V = \frac{(\omega_B+\omega_\parallel)^{3/2}(\omega_\parallel-\omega_\perp)}{\omega_B\sqrt{\omega_\parallel}} + \frac{4(\omega_B+\omega_\parallel)^2(\omega_\parallel-\omega_\perp)a}{\pi^{3/2}\omega_\parallel\omega_B^2 a_\parallel}. \tag{2}$$

In Fig. 3(a) we study the behavior in a trap with ellipticity $\omega_\perp = 0.5\omega_\parallel$ and $\omega_B = 5\omega_\parallel$. In the noninteracting system the crossover between longitudinal and transverse states predicted by exact diagonalization is at $V \approx 1.87\omega_\parallel$ that is in good agreement with the perturbation theory estimate $V \approx 1.46\omega_\parallel$. The critical barrier height falls with rising interaction strength due to the inhomogeneous pairing pulling density onto the central barrier and so favoring the longitudinal mode that has a node over the barrier. With spherically symmetric pairing this transition would be independent of interaction strength so its gradient exposes the inhomogeneous pairing. The transition could be exposed by starting from four trapped atoms and tilting the trap so that one atom escapes, with the other three atoms entering the ground state. The tunneling rate, proportional to ground state degeneracy, will be twice as large for the transverse mode as the longitudinal, thus mapping the boundary.

As demonstrated in Fig. 1 the atoms can bind into a singly degenerate Bose-Einstein condensate with s-wave symmetry. This gives the molecular ground state in Fig. 3(a). At $V = 0$ this occurs at $a_\parallel/a = 2.86$, which is greater than the $a_\parallel/a = 2.17$ for the spherically symmetric system due to the lower energy cost of occupying the transverse state. The critical interaction strength is at a minimum at the boundary between the transverse and longitudinal states at $V \approx 1.2\omega_\parallel$ since those two states are most unstable here. The transverse state is more stable as the central barrier is reduced, whereas the molecule with density sited over the barrier becomes less favorable with increasing barrier height than the longitudinal mode that has a node over the barrier. Systems containing more atoms will display analogous phase behavior governed by their symmetries that were studied earlier.

Discussion.—The few trapped fermions pose a nexus between analytically tractable few-body physics and intractable many-body systems. We have studied the imbalanced superfluid whose ground state displays inhomogeneous pairing. The pairing is analogous to the elusive LO state with the unpaired majority spins residing along the nodes of the pairing order. The $|2,1\rangle$ atoms possess a simple pairing topology that couples to the trap ellipticity and central barrier that can be probed experimentally. The ground state of more atoms can be understood in terms of the excited states of

the $|2, 1\rangle$ system. Moreover, the system approaches the infinite-body limit when more than eight atoms are trapped, so our study has broad implications for the FFLO phase.

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