Concomitant modulated superfluidity in polarized Fermi gases

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Recent ground-breaking experiments studying the effects of spin polarization on pairing in unitary Fermi gases encountered mutual qualitative and quantitative discrepancies which seem to be a function of the confining geometry. Using numerical algorithms we study the solution space for a three-dimensional fully self-consistent formulation of realistic systems with up to 10^5 atoms. A study of the three types of solutions obtained demonstrates a tendency toward metastability as the confining geometry is elongated. One of these solutions, which is consistent with Rice experiments at high trap aspect ratio, supports a state strikingly similar to the long sought Fulde-Ferrel-Larkin-Ovchinnikov state. Our study helps to resolve the long-standing controversy concerning the discrepancies between the findings from two different experimental groups and highlights the versatility of actual-size numerical calculations for investigating inhomogeneous fermionic superfluids.

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I. INTRODUCTION

Superfluidity in a system of fermionic particles occurs when bosonic degrees of freedom emerge and condense via pairing of fermions. Understanding the strength of this pairing mechanism is closely tied to the search for high-temperature superconductors. A central issue that has animated this quest is the following: What happens to the pairs when the participating species have mismatched Fermi surfaces? Such a scenario occurs, for example, in the presence of a polarizing field, or when the pairing species have unequal numbers or masses. The issue is that, when the mismatch of the Fermi surface is large enough, a competition between a normal polarized state and the superfluid state would ensue [1,2], potentially giving rise to yet unknown or poorly understood exotic superfluid states [3]. Among the interesting theoretical proposals for s-wave pairing is the Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) state, a collective term for an inhomogeneous superfluid referring either to a Fulde-Ferrell (FF) state [4], which supports a supercurrent, or a Larkin-Ovchinnikov (LO) state [5] with a spatially modulated order parameter. Other proposals include breached pairing and p-wave symbiotic superfluids [3]. Primarily due to lack of sufficient experimental evidence, the issue remains largely unresolved even though it is central to many forms of matter such as superconductors, neutron stars, and color superfluids in the quark-gluon plasma [3]. Ultracold samples of two-component degenerate Fermi gases [6–10] have re-energized the debate because of their exquisite controllability.

In this paper, we focus on apparently contradictory results on spin-imbalanced unitary Fermi gases from recent experiments between two leading groups [7–10]. In both experiments it was observed that, consistent with earlier predictions [1,2], the trapped superfluid responds to polarization by phase separating into an inner core with negligible polarization surrounded by a polarized outer shell. However, in the Rice experiments [8,9], performed in cigar-shaped traps with total particle numbers $N \sim 10^5$, a significant and unexpected deformation of the central superfluid core was observed, indicating a clear violation of the local density approximation (LDA). In addition, these results also suggest a much higher superfluid to normal (Chandrasekhar-Clogston) transition than in the MIT experiments [7,10] in which no deformations were observed. The excellent quantitative agreement with theory [11,12] for the MIT experiments, conducted at much lower trap aspect ratio and with higher particle numbers $N \sim 10^6$, hints that there might be unexpected physics at work in the Rice experiment. In addition, the concurrence of experiments performed in Paris [13] with the MIT experiments also suggests a crucial role of the trapping geometry. This impasse has inspired speculation about the possible role of exotic phases such as the FFLO state in the observed discrepancies and stirred much discussion and debate over the past few years by the cold-atom community.

The apparent contradiction between the Rice and MIT experiments reflects theoretical difficulties within trapped geometries: Since the effective chemical potential (μ) varies in space, several phases may coexist within a trapped sample. Consequently, despite excitement and considerable effort, the theoretical complexity inherent within the problem has ensured that most treatments have, with few exceptions [14–18], invoked the LDA [19,20], which is not general enough to capture states such as the FFLO. Although an intriguing LDA treatment which phenomenologically includes a surface energy correction has been able to account for the shape of the distortions [21], further studies reveal that this model is not consistent with a microscopic calculation of the surface tension [22]. On the other hand, recent studies employing variational techniques in isotropic geometries [23,24] have shown that the region of stability for the FFLO state is much larger than originally predicted [25]. Until now, a fully self-consistent treatment in anistropic geometries with realistic particle numbers has been well out of reach despite its relevance here and in a wide variety of other physical systems. To surmount this problem, we developed scalable numerical techniques which take full advantage of today's high-performance computing facilities running parallel codes over thousands of CPUs.

II. MODEL

We consider a gas of spin-polarized fermionic atoms confined to a harmonic trap defined in cylindrical coordinates (r,ϕ,z) by $V(r,\phi,z) = \frac{m}{2}(\omega_\perp^2 r^2 + \omega_z^2 z^2)$ with axial and radial frequencies denoted by $(\omega_z,\omega_\perp)$. Consistent with Refs. [8,9] we work at the unitarity limit where the s-wave scattering length between the two spin species (a_s) diverges and within a cigar-shaped trap with aspect ratio defined by $\alpha = \omega_\perp/\omega_z$. This system of $N = N_\uparrow + N_\downarrow$ atoms is described by a Hamiltonian $\hat{H} = \int d\vec{r}\,(\hat{H}_0 + \hat{H}_I)$ with noninteracting ($\hat{H}_0$) and interaction ($\hat{H}_I$) energy densities given by

$$\begin{aligned}\hat{H}_0(\vec{r}) &= \sum_{\sigma=\uparrow,\downarrow} \psi_\sigma^\dagger \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r,z) - \mu_\sigma \right] \psi_\sigma, \\ \hat{H}_I(\vec{r}) &= -U\, \psi_\uparrow^\dagger(\vec{r})\psi_\downarrow^\dagger(\vec{r})\psi_\downarrow(\vec{r})\psi_\uparrow(\vec{r}),\end{aligned} \tag{1}$$

where $\psi_\sigma(\vec{r})$ and $\psi_\sigma^\dagger(\vec{r})$ represent the fermionic field operators, m is the mass, and μ_σ is the chemical potential of atomic species with spin σ. Henceforth, we work in trap units for which $m = \omega_z = \hbar = 1$. The bare coupling constant U is renormalized through a relationship with a_s by $1/U = -1/(4\pi a_s) + (1/V_l)\sum 1/(2\epsilon_k)$ [12,26], with $\epsilon_k = k^2/2$ and V_l representing the system volume. $\hat{H}$ is diagonalized through the Bogoliubov-de Gennes (BdG) formulation. In particular, our formulation is identical to that in Ref. [12]. The superfluid gap (order parameter) is defined by $\Delta(\vec{r}) = U\langle\psi_\uparrow(\vec{r})\psi_\downarrow(\vec{r})\rangle$ and the spin densities are given by $\rho_\sigma(\vec{r}) = \langle\psi_\sigma^\dagger(\vec{r})\,\psi_\sigma(\vec{r})\rangle$. We find it clarifying to express our results in terms of the Fermi energy $E_F = (3N)^{1/3}\alpha^{2/3}$ and the Thomas-Fermi radius along the z axis, $Z_F = \sqrt{2E_F}$, for a single-species ideal Fermi gas of $N/2$ particles in a trap with identical parameters. In addition, following a convention that $N_\uparrow > N_\downarrow$, we define $k_F^{\uparrow\downarrow} = \sqrt{2\mu_{\uparrow\downarrow}}$ and the FFLO wave number by $q_0 = k_F^\uparrow - k_F^\downarrow$.

III. RESULTS AND DISCUSSIONS

We solve the BdG equations [12] using a piecewise-linear finite-element basis which yields sparse matrices amenable to efficient parallelization and work in a canonical formalism which fixes N and the total polarization $P = (N_\uparrow - N_\downarrow)/N$. It has been recently shown that, in the particular circumstances of the Rice experiment [8,9], evaporative cooling shortens the major axis (z axis) of what should be an ellipsoidal partially polarized region, where the condensate forms [27]. By starting from an initial ansatz for the gap (Δ_I) imitating this circumstance, the BdG equations are iteratively solved to self-consistency using a modified Broyden's method [28]. Our calculations reveal the following: (1) For large particle numbers ($N \gtrsim 10^4$), we always find a solution similar in structure to the LDA solution which has the lowest free energy. However, starting from an axially shortened initial ansatz for the gap, this solution is not accessed by the iterative procedure. (2) The most likely solution which is consistent with the Rice experiment is a metastable state that supports a partially polarized superfluid phase strikingly similar to the FFLO phase. This state becomes increasingly robust as trapping geometry becomes more elongated. (3) Even within a trapped environment, the nodes of the order parameter in the FFLO-like phase are radially aligned, which, with low enough noise, provides a measurable, incontrovertible signal within the density profiles.

Superfluidity, a phenomenon of quantum rigidity, acquires its name from a scenario in which, due to energy barriers, a condensate gets indefinitely trapped within a current-carrying metastable state. The portent for the experiments under discussion is that the observed state could be a long-lived metastable state. Thus, we take the approach of exploring the solution space using an ansatz constructed with reference to [27] and the phase diagram on the BCS side of the Feshbach resonance [25,29]. Specifically, we use the LDA solution for the gap ($\Delta_{\rm LDA}$) as a base to construct an initial ansatz Δ_I which is axially partitioned into different regions:

$$\Delta_I(r,z) = \begin{cases} \Delta_{\rm LDA}, & |z| < z_c, \\ \Delta_{\rm LDA}\cos[q(z - z_c)]\, e^{-(z-z_c)^2/\lambda^2}, & |z| > z_c. \end{cases}$$

Δ_I allows us to explore various distorted states. In its most general form, one encounters the unpolarized BCS, FFLO, and normal phases as one traverses along the axial direction from the trap center to the edge. The initial size of the FFLO region in the ansatz is determined by λ. When λ is too small to accommodate a single wavelength of the gap oscillation, i.e., $0 < \lambda < 2\pi/q$, we start without an FFLO phase and z_c represents the axial coordinate of superfluid to normal (S-N) transition. Conversely, an FFLO phase is initially present in the ansatz when $\lambda > 2\pi/q$. In this case z_c represents the superfluid to FFLO (S-FFLO) transition. Henceforth we refer to these initial conditions as $\Delta_I^{\text{P-N}}$ and $\Delta_I^{\text{P-SF}}$, respectively, which reflects our nomenclature for the eventual solutions as well; i.e., we name the entire solution according to the character of the partially polarized region: We have a partially polarized superfluid solution (P-SF) when there is an FFLO-like phase present. When the partially polarized region is completely normal, we refer to the entire solution as a P-N solution. For clarity we single out the LDA-like solution which is obtained when $\Delta_I = \Delta_{\rm LDA}$ as the SF solution. In both the P-N and P-SF solutions, the central unpolarized BCS superfluid core is shortened along the z axis in comparison to the LDA-like SF solution. As we shall see, this shortened BCS core is manifested in the LDA-violating distortion of the density profile of the minority spin component.

A broad feature of our results, which directly relates to the question of metastability, is the observation of a barrier between the shortened states (either P-N or P-SF) and the SF solution. For small atom numbers, this barrier is absent, the converged solution is unique, independent of the initial ansatz we take, and we see a dramatic departure from the LDA prediction due to significant finite-size effect. However, with increasing N, the axial S-N or S-FFLO transition point is pinned near its initial value z_c and we obtain different solutions by starting from different initial ansatzes. Starting from $\Delta_I^{\text{P-SF}}$ or $\Delta_I^{\text{P-N}}$ we always converge to a shortened state in a manner which is *only* sensitive to our choice of q. In other words, we do see a transition between the P-SF and P-N states which is very sensitive to q and largely insensitive to λ, both of which are set in the initial condition Δ_I. It works as follows. When q is less than a critical value q_c, the oscillations in the ansatz Δ_I are amplified and the solution flows to a P-SF state regardless of the size of λ. Conversely, when $q > q_c$, the oscillations are damped and Δ_I always converges to a P-N state. A similar resonance behavior has also recently been observed in studies of the S-N boundary while tuning a_s across the BEC-BCS crossover [22], in which case calculations were

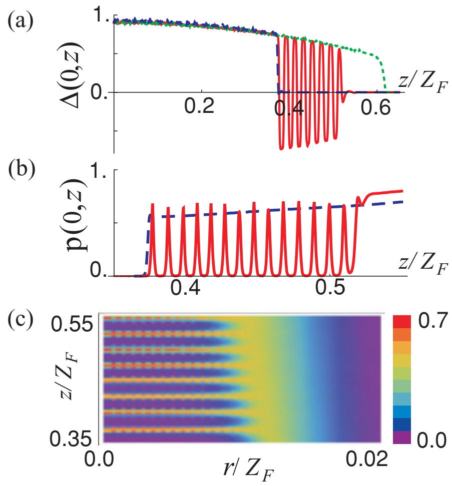

FIG. 1. (Color online) (a) Axial profiles of the gap (in units of E_F) showing the P-N (blue dashed line), P-SF (red solid line) and SF (green dotted line) states. The LDA solution (not shown) almost completely overlaps with the SF result. The free energies per particle are: $0.67(0)E_F$, $0.65(8)E_F$, $0.65(5)E_F$ and $0.64(4)E_F$ for the P-N, P-SF, SF and LDA states, respectively. (b) Local polarization $p(\vec{r})$ within the partially polarized region of the P-SF(red solid line) and P-N(blue dashed line) solutions. (c) An r-z plot of the normalized density difference $\delta\rho = (\rho_\uparrow - \rho_\downarrow)/\rho_F$ of the partially polarized region of the P-SF state ($\rho_F = \sqrt{(2E_F)^3}/6\pi^2$). All the results shown in this paper are obtained at a small temperature $T = 0.02E_F/k_B$, and with $N = 50\,000$, $\alpha = 50$, and $P = 0.3$.

performed without the radial confinement. It is possible that this phenomenon might be exploited to engineer the realization of the P-SF state.

We ascribe the consistent convergence to a shortened state as due to the emergence of energy barriers separating the P-SF and P-N states from the SF state with increasing N or α in tandem with E_F. In Fig. 1(a) we illustrate the dramatic differences in the superfluid gap for the various solutions encountered. Apart from the emerging energy barriers, another important result with regard to metastability is the decrease in the relative energetic separation of all the states, P-SF, P-N, and SF, as α is increased. Taken together, these observations suggest that the relaxation of the physical system from any of the shortened states to the SF state, which is the lowest in energy, becomes *less* favorable as α is increased, a deduction which is borne out by the discrepancies of the Rice and MIT experiments.

For a given value of z_c, the energy of the P-SF solution is consistently lower than the P-N solution. Furthermore, recent results suggest that the inclusion of fluctuations, neglected in mean-field formulations, should make the P-SF state even more stable [24]. Thus, we expect that if the system converges to a shortened state, it will choose the P-SF state. A natural question to ask is, How will the FFLO phase manifest itself?

In Fig. 1(b) we contrast the appearance of local polarization $p(\vec{r}) = (\rho_\uparrow - \rho_\downarrow)/(\rho_\uparrow + \rho_\downarrow)$ in the partially polarized regions of the P-SF and P-N states. We note that, in [24], the strong oscillations displayed in $p(\vec{r})$ were observed to survive the effects of fluctuations. One pleasant surprise of our results

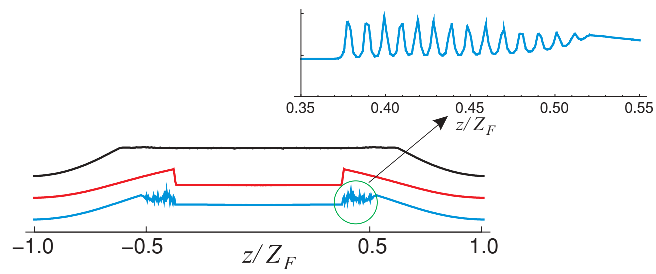

FIG. 2. (Color online) Plots showing the doubly integrated axial spin density $\delta\rho_{1d}(z)$ for, from top down, the SF, P-N, and P-SF states shown in Fig. 1(a).

was the radial alignment of the nodes of the FFLO phase shown in Fig. 1(c), a fact which is not *a priori* obvious and is very promising for the prospects of detection within the three-dimensional (3D) system under discussion here, because it implies that the FFLO phase could yield a measurable signal in the density profile. Auspiciously, it also suggests that when an array of one-dimensional (1D) tubes, such as are being used in current experiments [30], are coupled to yield a quasi-3D confinement, the FFLO nodes at each tube are likely to align to yield a measurable signal. To make sure that the radial alignment of the nodes is not a numerical artefact, we have used initial an ansatz where the nodes are intentionally misaligned along the radial direction. Our code always converges to states with the nodes aligned. A comparison of the plots in Fig. 2 confirms that the presence of an FFLO phase would indeed provide a smoking-gun signal in doubly integrated axial spin density $\delta\rho_{1d} = \int\int dxdy(\rho_\uparrow - \rho_\downarrow)$. In the close-up we observe that the signal of the FFLO region is not as strong as that in Fig. 1(c) because of contributions from the fully polarized shell encasing it. Quantitatively, it indicates that a lower bound of the signal to noise ratio of ≈ 6.5 is required to observe at least half of the FFLO phase.

A casual comparison of all column density profiles in Fig. 3 rules out the observation in the Rice experiment of the SF state, which is consistent with the LDA and, within the BdG formulation, has the lowest free energy. However, due to the noise on the experimental data, it is not clear which of the shortened states (P-SF or P-N) has been observed. To produce noise with characteristics similar to that of the experiment, we added white noise with a standard deviation that is a similar fraction of the average value of the column density

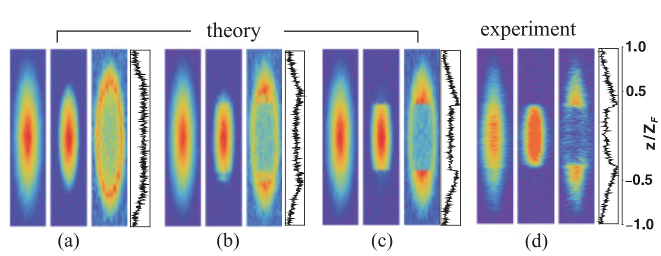

FIG. 3. (Color online) Column densities (rescaled to have aspect ratio 5 for clarity) $\int \rho_\uparrow dx$, $\int \rho_\downarrow dx$, and $\int(\rho_\uparrow - \rho_\downarrow)\,dx$ and the axial spin density $\delta\rho_{1d}$, respectively. The states represented are (a) the SF, (b) the P-SF, and (c) the P-N states illustrated in Fig. 1(a). In (d) we plot the Rice experimental results for $N \approx 260\,000$, $P \approx 0.35$, $\alpha = 45.23$, and $T < 0.05E_F/k_B$.

$\int_{-\infty}^{\infty} \rho_\uparrow \, dx$ in the plotted window. Theoretically, since it has the lower energy and since the transition between the FFLO phase and the normal phase is continuous, one expects that, between the two shortened states, the P-SF solution will be favored.

IV. CONCLUSION

In conclusion, we have repeatedly solved the BdG equations in a cigar-shaped trap using initial conditions which imitate the condensate nucleation process [27]. The iterative solution chooses between two stationary points, which are not necessarily the global free energy minimum, each of which features density profiles strikingly similar to experimental observations at Rice. The solution which possesses the lower energy of these two contains an FFLO-like phase which leaves an accessible signal in $\delta\rho_{1d}$. Coupled with recent results which suggest the unexpected stability of the FFLO in three dimensions [24], our observations raise the interesting question of whether the FFLO state has already been realized in the Rice experiment. Since the Hartree interactions are excluded from the BdG formulation of unitary gases [12], we do not address the position of the Clogston limit. Nevertheless, we note in passing that the P-SF solution has the capacity to absorb polarizations and, if undetected, could conceal the existence of a partially polarized region. Finally, we remark that our work is important for another reason: As far as we know ours are among the largest calculations of their kind and provide an efficient tool for investigations of finite fermionic systems such as occur in atomic traps or in nuclear physics, where predictions of ideal models such as the FFLO proposal could be significantly modified by confinement and finite-size effects.

Note added. After our work was completed, the Rice experimental group verified the suggestion made in Ref. [27] that the LDA-violating deformations observed in their experiment are a result of depolarization of the superfluid core by evaporation occurring mainly at the axial center of the trap [31]. They found that these deformed states are very stable, in agreement with our calculations. The metastability of these states suggests the possibility to directly engineer an FFLO state in an elongated trap.

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