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Competition between Normal Superfluidity and Larkin-Ovchinnikov Phases of Polarized Fermi Gases in Elongated Traps

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By applying the recently proposed antisymmetric superfluid local density approximation (ASLDA) to strongly interacting polarized atomic gases at unitarity in very elongated traps, we find families of Larkin-Ovchinnikov (LO) type of solutions with prominent transversal oscillation of pairing potential. These LO states coexist with a superfluid state having a smooth pairing potential. We suggest that the LO phase could be accessible experimentally by increasing adiabatically the trap aspect ratio. We show that the local asymmetry effects contained in ASLDA do not support a deformed superfluid core predicted by previous Bogoliubov-de Gennes treatments.

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The *s*-wave pairing in two-component fermion systems is the most common mechanism inducing superconductivity or superfluidity in the realm of condensed matter, nuclear physics, and cold atom gases [1]. The latter system, that was experimentally realized in recent years [2–6], has the great advantage that the pairing strength can be manipulated using Feshbach resonances to access the whole range of the BCS to BEC crossover. The competition between *s*-wave pairing strength, trap deformation, population imbalance, and temperature could give rise to different superconducting phases and regions of phase separation. Recent experiments with two-component polarized ultracold atomic gases in elongated traps open the possibility of the practical realization of long-sought exotic superfluid phases. Among them, the Fulde-Ferrer (FF) [7] state representing a condensate of Cooper pairs with a finite center-of-mass momentum and the Larkin-Ovchinnikov (LO) [8] state with a spatially oscillating pairing potential have attracted much interest [9, 10].

The Rice experiment [5] on a polarized unitary gas has been at the center of an intense debate. They observed a spherical distortion of the superfluid core shape with respect to the elongated trap with an aspect ratio $\eta \sim 50$. Such a shape mismatch was not observed in the MIT experiment performed with a much less elongated trap ($\eta \sim 5$) [4]. Recent experiments performed in traps of $\eta \sim 22$ [6] seem to confirm the MIT results. These seemingly conflicting experimental results have motivated significant theoretical efforts [11–14].

Most of the theoretical approaches to trapped cold atoms have been based on the Local Density Approximation (LDA) or in the Bogoliubov-de Gennes mean-field approximation (BdG) with a contact interaction. These approximations, which are appropriate in the weak-coupling BCS region, are not expected to perform well in the strongly interacting region due to in-medium screening effects. However, most of the experiments are accomplished for strongly coupled dilute fermionic superfluids in the unitary limit in which the *s*-wave scattering length approaches infinity ($|a_s| \to \infty$). In this limit, the system exhibits universal behavior governed by the densities, making it ideally suited for a density functional theory (DFT) description [15–17]. DFT offers a way to incorporate experimental information, and the results of large-scale calculations like Monte Carlo [18, 19] within an accurate energy density able to describe strongly interacting systems due to the incorporation of many-body effects.

Recently, SLDA [15, 16], a superfluid extension of DFT, was applied to symmetric two-component systems. Subsequently, it was generalized to polarized fermionic systems (ASLDA) [20], finding strong evidence for the existence of a stable LO phase in the thermodynamic limit. The LO phase was predicted to be stable in large regions of the parameter space of a polarized one-dimensional (1D) system [21], and very recently experimental evidence for a LO phase has been obtained in a spin mixture of ultracold ^{6}Li atoms trapped in an array of 1D tubes [22]. Extremely elongated traps offer, therefore, a unique opportunity to explore the transition from 3D to 1D polarized systems, and the competition between normal and exotic superfluid phases as a function of the aspect ratio.

In this work we study cold polarized atoms in elongated traps at unitarity. The self-consistent BdG equations of superfluid DFT are solved using the coordinate-space axial solver HFB-AX [23, 24], based on B-splines, which has been demonstrated to provide precise results at large deformations. In a previous work [23] we showed the appearance of phase separation in deformed SLDA. Here, we compare SLDA results with those of the ASLDA formalism that has been tailored to describe imbalanced systems. Our focus is on phase separation effects, deformation of superfluid cores, and the appearance of superfluid oscillating phases for different trap elongations.

The grand-canonical energy density functional of ASLDA can be written as [20]

$$\mathcal{E} = \sum_{\sigma=\uparrow,\downarrow} \left(\alpha_\sigma(x)\frac{\tau_\sigma}{2} - \lambda_\sigma \rho_\sigma \right) + \frac{(3\pi^2\rho)^{5/3}}{10\pi^2}\beta(x) - \Delta\kappa, \quad (1)$$

where the densities of spin-up $\rho_\uparrow(\boldsymbol{r})$ and spin-down $\rho_\downarrow(\boldsymbol{r})$ atoms, the pairing densities $\kappa(\boldsymbol{r})$, and pairing gaps $\Delta(\boldsymbol{r})$ are:

$$\begin{aligned} \rho_\uparrow(\boldsymbol{r}) &= \sum_i f_i |u_i(\boldsymbol{r})|^2, \; \rho_\downarrow(\boldsymbol{r}) = \sum_i (1-f_i)|v_i(\boldsymbol{r})|^2 \\ \kappa(\boldsymbol{r}) &= \sum_i f_i u_i(\boldsymbol{r}) v_i^*(\boldsymbol{r}), \; \Delta(\boldsymbol{r}) = -g_{eff}(\boldsymbol{r})\kappa(\boldsymbol{r}), \end{aligned} \quad (2)$$

and $\rho = \rho_\uparrow + \rho_\downarrow$. In Eqs. (1-2), $f_i = 1/(1+\exp(E_i/kT))$, $u_i(\boldsymbol{r})$ and $v_i(\boldsymbol{r})$ are eigenvectors of the BdG Hamiltonian, and E_i is the corresponding eigenvalue. The BdG equations are solved self-consistently with the chemical potentials λ_σ (σ=$\uparrow,\downarrow$) being determined from the particle-number constraints N_σ=Tr(ρ_σ) [12, 25], where $N_\uparrow$ ($N_\downarrow$=$N - N_\uparrow$) is the number of spin-up (spin-down) fermions. The local polarization is given by $x(\boldsymbol{r}) = \rho_\downarrow(\boldsymbol{r})/\rho_\uparrow(\boldsymbol{r}) \leqslant 1$ while the total polarization of the system is P=$(N_\uparrow - N_\downarrow)/N$. The quantities $\alpha_\sigma(x)$ and $\beta(x)$ that parametrize the local effective masses and normal interaction, respectively, were fitted to Monte Carlo data and experiment [20].

The minimization of the energy density (1) leads to a BdG set of equations:

$$\begin{bmatrix} h_\uparrow(\boldsymbol{r}) - \lambda_\uparrow & \Delta(\boldsymbol{r}) \\ \Delta^*(\boldsymbol{r}) & -h_\downarrow(\boldsymbol{r}) + \lambda_\downarrow \end{bmatrix} \begin{bmatrix} u_i(\boldsymbol{r}) \\ v_i(\boldsymbol{r}) \end{bmatrix} = E_i \begin{bmatrix} u_i(\boldsymbol{r}) \\ v_i(\boldsymbol{r}) \end{bmatrix} \quad (3)$$

where the single-particle Hamiltonian $h_\sigma = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\alpha_\sigma) + U_\sigma + V_{\rm ext}$ depends on the kinetic term, Hartree potential U_σ, and external harmonic trap potential $V_{\rm ext}$. The ASLDA equations are solved with a finite energy cutoff E_c ($|E_i| \leqslant E_c$) and a local regularized pairing interaction $g_{eff}(\boldsymbol{r}) = \gamma[\rho^{1/3}(\boldsymbol{r}) + \Lambda(\boldsymbol{r})\gamma]^{-1}$ [16], where γ is the original pairing interaction, and $\Lambda(\boldsymbol{r})$ is the average regulator for the spin-up and spin-down components. The SLDA formalism can be obtained from ASLDA assuming $x(\boldsymbol{r}) = 1$, resulting in identical effective masses and Hartree potentials for spin-up and spin-down species. The potential of the confining trap is $V_{\rm ext}(\mathbf{r}) = \frac{\omega^2}{2}(r^2 + z^2/\eta^2)$, where η is the aspect ratio defining the trap elongation. The ASLDA equations are solved with HFB-AX in a discretized rectangular axial box (r, z). We work in trap units for which $\hbar = m = \omega = 1$. The energy cutoff was assumed to be $E_c > 5\lambda_\uparrow$ (in practice, it was 35 in SLDA and 25 in ASLDA).

We first study the occurrence of multiple superfluid solutions predicted in a BdG treatment of large-scale

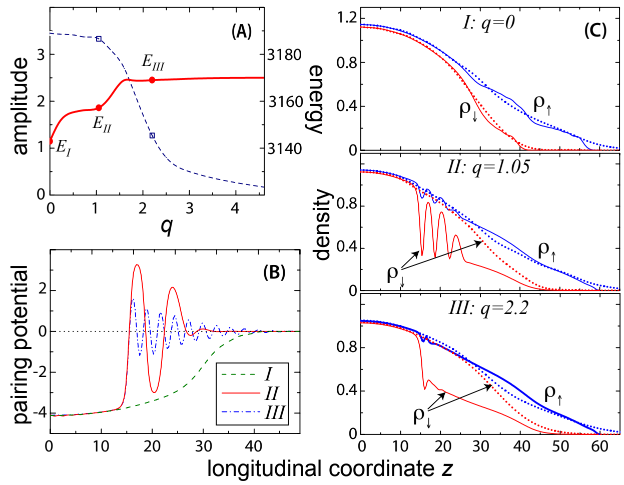

FIG. 1: (Color online) SLDA results for a system of 1000 atoms in a trap with aspect ratio η=20 and polarization of P=0.37. (A) Energies of various self-consistent solutions of SLDA obtained by starting from oscillating initial conditions with different values of q (solid line). For each solution, the amplitude of the first oscillation in the pairing potential is shown (dashed line). (B) Pairing potentials for the three solutions with q=0 (I), q=1.05 (II), and q=2.2 (III). (C) Density profiles $\rho_\uparrow$ and $\rho_\downarrow$ for the cases (I-III) along z (longitudinal direction; $r = 0$, solid line) and ηr (transverse direction; $z = 0$, dotted line). Large deviations between longitudinal and transverse profiles are indicative of deformation effects. If solid and dashed profiles are close, density distributions follow the geometry of the trap. See text for more details.

trapped systems [11]. Similar to Ref. [11], we parameterize an initial guess for the pairing potential along the z-axis as $\sin[q(z - z_c)]e^{-(z-z_c)/\xi}$, where z_c is the critical distance at which oscillations develop. Figure 1 displays SLDA results for N=1000 atoms with polarization P=0.37 in a trap with η=20. (It was advantageous to use SLDA in this systematic study of various self-consistent solutions as this approach is less computationally intensive than ASLDA.) We performed systematic calculations with different values of the wave number q finding a multitude of self-consistent SLDA solutions. The panel A of Fig. 1 shows the energies of SLDA states as a function of q together with the amplitude of the first oscillation of the pairing potential. The ground-state (g.s.) solution has q=0. In the energy curve, one can see two plateaus, the first one with $0.4<q<1.1$ containing nearly degenerate solutions having large oscillation amplitudes and the second, with $q > 1.5$, containing nearly-degenerate solutions exhibiting low-amplitude oscillations. From them we select three typical solutions: (I) g.s. with q=0, (II) excited state with q=1.05, and (III) excited state with q=2.2. Panel B shows the corresponding pairing potentials along the z-axis and panel C displays the density profiles in longitudinal and transverse directions for the three states. Solution (II), with remarkable oscillations in the pairing potential and density profiles, is a LO state (see discussion below). The higher-energy state (III) does not show appreciable oscillations in the density profiles. Unlike the solution I, solution II and particularly solution III show the presence of the deformation effect in the minority component, similar to the one observed in the Rice experiment.

The presence of nearly degenerate solutions at very large elongations of the trap should not be surprising. Indeed, the trap excitation along the z-axis is $\Delta E_z = \hbar\omega_z/2 = 1/(2\eta)$. In the example of Fig. 1, $\Delta E_z = 0.025$, which is $\sim$0.5% of the Fermi energy. This means that the trap provides a quasi-continuum background of states with smoothly increasing energy and wave number. We note that the wave number of state (II) $q_{II} \approx q_{LO}$, where $q_{LO} = \sqrt{2\lambda_\uparrow} - \sqrt{2\lambda_\downarrow}$ is the LO wave number. All states belonging to the plateau around solution II have very similar values of chemical potentials, hence practically identical values of q_{LO}. This suggests that the LO can be represented by a superposition of the DFT solutions with q around q_{LO} [19]. Indeed, it is anticipated that the inclusion of quantum fluctuations beyond DFT could mix nearly degenerate solutions, thus lowering the energy of the LO state with respect to the ground state.

In Fig. 2 we compare density profiles in the longitudinal and transverse directions in SLDA and ASLDA for a g.s. configuration of 2000 polarized atoms with P=0.37 in a moderately elongated trap of η=10. The insets depict the pairing potential in the longitudinal direction. At this elongation, some low-amplitude oscillations in the pairing potential are present, but they are absent in the density profiles. By comparing the longitudinal and transverse density profiles, one can see a clear sign of deformation of the core in the SLDA solutions as predicted by the BdG calculations of Refs. [12, 14]. However, when the local polarization effects are considered in ASLDA, the superconducting core follows the shape of the trap. Moreover, deformation effects in SLDA are washed out at temperatures around 20% of the Fermi temperature, see Fig. 2.

Starting from the g.s. ASLDA solution at η=10, we evolve it gradually by increasing the aspect ratio. In this way we can reach an excited state of the system with q>0. The resulting two-dimensional pairing potentials for η=20, 30, and 40 are shown in Fig. 3. Figure 3 shows that the oscillations in the pairing potential, already present for η=20, grow dramatically with the aspect ratio. The fact that the oscillations have transversal character (are radially aligned), also seen in large scale BdG calculations [11], gives another support for identifying this solution as a LO state. Moreover, the strengthening of the oscillations at higher aspect ratios is consistent with the expectation of a LO phase in the quasi-1D limit [10, 21, 22]. The numerical procedure for the solution of ASLDA may simulate an experimental process in

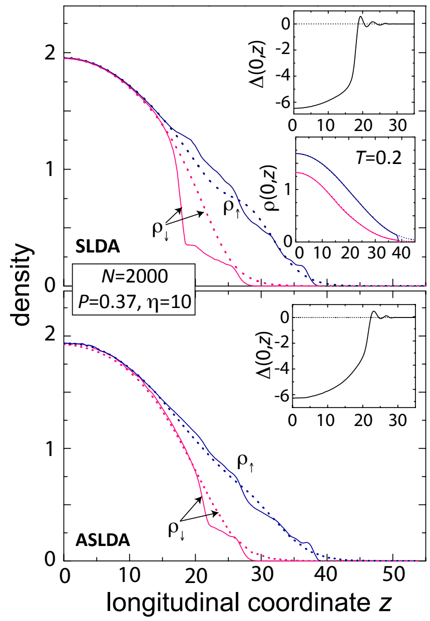

FIG. 2: (Color online) Density profiles for the g.s. configuration in SLDA (top) and ASLDA (bottom) in the longitudinal (solid lines) and transverse (dashed lines) directions. The pairing potentials Δ and the SLDA density profiles at temperature T=0.2 are shown in the insets.

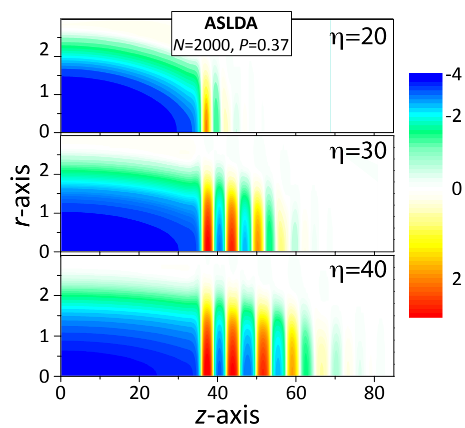

FIG. 3: (Color online) Pairing potential $\Delta(r, z)$ evolved from the ASLDA g.s. solution of Fig. 2 to aspect ratios η=20 (top), 30 (middle), and 40 (bottom). The radial alignment of the nodes, characteristic of the LO state [11], is clearly seen. The LO wave numbers are q_{LO}=1.32, 1.18, and 1.13 for η=20, 30, and 40, respectively. Note the different scales in z and r.

which a polarized atomic gas is formed in a moderately elongated trap and then the aspect ratio is increased adiabatically to high elongations.

In order to gain a deeper insight into the ASLDA formalism, we show in Fig. 4 density profiles, Hartree potentials U_σ, and effective masses α_σ^{-1} in the longitudinal direction for the two atomic species in a trap of aspect ratio η=30 and P=0.37. All these quantities exhibit pro-

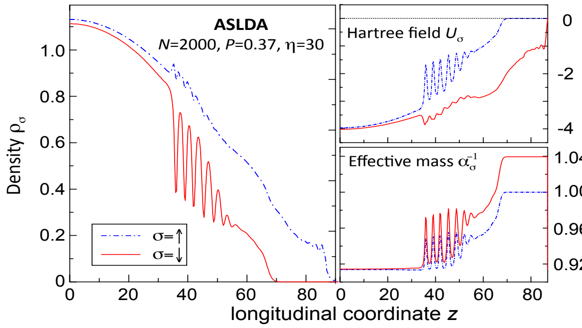

FIG. 4: (Color online) Densities, Hartree potentials, and effective masses for an excited ASLDA state of 2000 atoms with P=0.37 in a trap with η=30. The solid and dashed-dotted lines indicate the spin-up and spin-down components, respectively.

nounced oscillations consistent with the oscillations in the pairing potential of Fig. 3. Unlike in the SLDA formalism, these oscillations are very different for the two species. The Hartree potential, usually neglected in BdG calculations, has a significant influence on the self-consistent ASLDA solution. The rather shallow Hartree potential of the spin-down component does not favor the deformed-core solution, explaining the different density shapes seen in SLDA and ASLDA in Fig. 2. In these calculations, we used a large box with $z_{\max}$=90. We checked, however, that our results for profiles inside the box, are numerically stable with respect to small variations in $z_{\max}$. Another interesting feature is that the effective masses, fitted to Monte Carlo calculations, are different at the trap boundaries. A recent experiment [6] estimated the effective mass of the Fermi polaron to be 1.17(10), while it was fitted to be 1.04 in Ref. [20]. Our calculations with the new effective mass do not change appreciably from the presented ASLDA results.

In summary, we have performed precise superfluid-DFT studies of spin-imbalanced Fermi gases in elongated traps at unitarity. Calculations using initial conditions with different pairing oscillations yield families of coexisting pairing phases: the LDA solution characterized by a smooth pairing potential and LO type of solutions characterized by transversal oscillation of pairing potential in the area of phase separation. In a theory beyond BdG, such as the multireference DFT, these LO states can be viewed as superpositions of DFT solutions with different q-values. The deformed-core solutions predicted in SLDA for g.s. configurations of polarized systems in moderately elongated traps are absent in ASLDA. Consequently, the presence (or absence) of such states in experiment might provide clues about the effective interaction in strongly interacting polarized atomic gases. Our results suggest that LO could be studied experimentally by elongating the traps adiabatically, starting from a moderately elongated equilibrium state.

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