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Published in:
Physical Review Letters

DOI:
[10.1103/PhysRevLett.106.095301](https://doi.org/10.1103/PhysRevLett.106.095301)

Published: 04/03/2011

Document Version
Publisher's PDF, also known as Version of record

Please cite the original version:

Kim, D.-H., Kinnunen, J. J., Martikainen, J.-P., & Törmä, P. (2011). Exotic superfluid states of lattice fermions in elongated traps. *Physical Review Letters*, 106(9), 1-4. [095301].
<https://doi.org/10.1103/PhysRevLett.106.095301>

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Exotic Superfluid States of Lattice Fermions in Elongated Traps

D.-H. Kim,¹ J. J. Kinnunen,¹ J.-P. Martikainen,² and P. Törmä^{1,*}

¹*Department of Applied Physics, Aalto University, P.O. Box 15100, 00076 AALTO, Finland*

²*NORDITA, 106 91 Stockholm, Sweden*

(Received 11 October 2010; revised manuscript received 4 December 2010; published 28 February 2011)

We present real-space dynamical mean-field theory calculations for attractively interacting fermions in three-dimensional lattices with elongated traps. The critical polarization is found to be 0.8, regardless of the trap elongation. Below the critical polarization, we find unconventional superfluid structures where the polarized superfluid and Fulde-Ferrell-Larkin-Ovchinnikov-type states emerge across the entire core region.

DOI: 10.1103/PhysRevLett.106.095301

PACS numbers: 67.85.-d, 03.75.Ss, 05.30.Fk, 71.10.Fd

The nature of pairing in spin-polarized fermion systems is a fundamental problem in many areas of physics, including superconductors in a strong magnetic field, neutron-proton pairing in nuclear matter, and color superconductivity in high density QCD [1–3]. Non-BCS pairing mechanisms have been proposed for spin-polarized fermions. The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) states exhibit finite-momentum pairing, causing spatially oscillating pair potentials [4,5]. In the polarized superfluid states, so-called Sarma or breached-pair states, zero-momentum pairing occurs, having excess unpaired particles [6–10]. In trapped ultracold Fermi gases [11,12], recent experiments with spin imbalance observed the superfluidity and the transition to the normal state with increasing polarization [13–16]. These systems offer an unprecedented access to the search for exotic superfluid states. In this Letter, we present the first large-scale calculations beyond mean-field theory, explicitly considering the trap geometry. We characterize the critical polarization of the transition and show evidence for exotic superfluidity.

The FFLO and polarized superfluid states have been originally proposed for translationally invariant systems. The FFLO state, in particular, has been suggested to be stabilized by reduced dimensionality. Therefore, it is important to incorporate broken translational symmetry caused by the presence of a trap in ultracold gases. Highly elongated traps were used in the experiments with spin-imbalanced ⁶Li gases [13–17]. Concerning previous mean-field theory calculations with explicit trap confinement [18], the FFLO-type oscillations have been expected to occur only at the narrow edges of the superfluid core in a spherical trap [19]. Quantum fluctuations are largely neglected in these mean-field calculations, and a full-scale *ab initio* approach remains elusive so far in three dimensions. Here we address this issue via an extension of dynamical mean-field theory considering both the full local quantum fluctuations and the trap effects.

We study the problem of a trapped lattice fermion system at zero temperature ($T = 0$) in three dimensions (3D) by using a *real-space* dynamical mean-field theory

(DMFT) [20–23]. With various trap aspect ratios examined for elongated traps, we find the critical polarization near 0.8 insensitive to the trap aspect ratios. In a wide range of polarizations, we observe that polarization and finite pair potential coexist at the core region, indicating the polarized superfluid core, surrounded by the normal unpaired particles. In highly elongated traps, as we approach the critical polarization, we find that the FFLO-type states emerge with spatially oscillating pair potential across the trap center. For comparison, we present also Bogoliubov–de Gennes (BdG) mean-field calculations.

Our real-space DMFT solves the attractive Hubbard model with an *anisotropic* trapping potential at $T = 0$,

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} (V_i - \mu_\sigma) n_{i\sigma},$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) a fermion with spin σ at site i , the density operator $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and μ_σ denotes the chemical potential. The hopping t between neighboring sites $\langle ij \rangle$ is set to unity. The on-site interaction U is chosen as the unitarity value for the cubic lattice, $U \simeq 7.915$ [24]. The trapping potential is given as $V_i = V_0[x^2 + y^2 + (z/\alpha)^2]$ where V_0 and α are the trap strength and aspect ratio. In the 3D lattice with size $L_x \times L_y \times L_z$, the coordinates of sites are assigned as $\xi' = \xi - \frac{1}{2}$, where $\xi \in \{x, y, z\}$, and $\xi = -\frac{L_\xi}{2}, \dots, \frac{L_\xi}{2} - 1$.

The real-space DMFT is constructed for inhomogeneous systems by considering local, yet site-dependent, self-energy terms, which explicitly include trap effects beyond the local density approximation (LDA). This approximation in the DMFT allows *s*-wave pairing [20]. The impurity problem now becomes site dependent and must be solved for each site with an efficient solver. We employ the exact diagonalization method to solve a 7-orbital impurity Hamiltonian with a superconducting bath [20] which provides a good convergence (cf. [25]) in our reliability tests. There are two advantages in choosing the exact diagonalization method: it is easy to consider the generalized Anderson model required to describe the superfluid phases;

it efficiently finds the ground state. The possible source of error is the effective bath of a limited number of orbitals, causing spiky spectral functions.

We consider harmonic trapping potentials with various trap aspect ratios $\alpha = 1, 2.5, 5, 7.5, 10$. The chemical potentials are adjusted to fix the total particle number $N = N_{\uparrow} + N_{\downarrow} \simeq 210$ with the polarization $P = (N_{\uparrow} - N_{\downarrow})/N$. The particle density is below quarter filling at all lattice sites. The trap strength is given as $V_0 = 0.02\alpha^{2/3}$ to keep the volume constant. The lattice size varies accordingly with α : $(L_x, L_y, L_z) = (24, 24, 24)$ for $\alpha = 1$, $(16, 16, 40)$ for $\alpha = 2.5$, $(16, 16, 40)$ for $\alpha = 5$, $(14, 14, 80)$ for $\alpha = 7.5$, and $(14, 14, 100)$ for $\alpha = 10$. The lattice size becomes a bottleneck in the real-space DMFT. The computation took $\sim 10^9$ CPU seconds in supercomputers.

Figure 1 shows how the distribution of particles and their superfluid characteristics change with polarization P in an elongated trap with aspect ratio $\alpha = 7.5$. The density difference $\delta n_i \equiv n_{i\uparrow} - n_{i\downarrow}$ and the pair potential $\Delta_i \equiv \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle$ characterize the superfluid structure: for small P 's, the particles at the trap center are fully paired superfluid (dark gray, $\delta n = 0$, finite Δ) and surrounded by unpaired particles (light gray, $\delta n \neq 0$). The small bumps in Δ are found along the axial (z) direction, which can be interpreted as an analog of the proximity effect at a superconductor-ferromagnet interface [26]. As P increases further, we find that two features become noticeable in Δ . For $P \gtrsim 0.7$, an oscillatory structure in Δ emerges across the trap center, indicating that FFLO-type states may exist

FIG. 1 (color online). Cross-sectional visualization of the particle density and pair potential structure in the elongated trap with the aspect ratio $\alpha = 7.5$ for selected polarizations $P \leq 0.8$. (a) The density difference $\delta n \equiv n_{\uparrow} - n_{\downarrow}$ is plotted in the $y = 0$ plane. The lighter (darker) gray indicates the larger (smaller) value of δn . Black defines $\delta n = 0$. (b) The pair potential $\Delta(x, y = 0, z)$ shows the evolution of the superfluid core structure as a function of P . The FFLO-like oscillations are observed at high P 's but below $P = 0.8$ where Δ vanishes.

in this elongated system. When P reaches 0.8, a transition to the normal phase occurs, as indicated by the complete suppression of Δ .

We study the transition to the normal phase systematically with the order parameter, $\eta \equiv \sum_i |\Delta_i|^2 / N_{\downarrow}$, averaged over the whole system. In Fig. 2(a), it turns out that the behavior of $\eta(P)$ and the critical polarization $P_c \simeq 0.8$ is *insensitive* to the trap aspect ratios that we have examined. Moreover, we find that our P_c agrees with $P_c \sim 0.78$ found in the experiments [15,16], and the quantum Monte Carlo (QMC) results in continuum with LDA [27,28]. The order parameter is comparable to the condensate fraction measured in [15].

On the other hand, we find that pairing in the superfluid core in our systems is unconventional. Figure 2(b) indicates the coexistence of finite polarization and order parameter at the center. This characterizes the polarized superfluid core and is apparent at intermediate or even at low P 's for large α . In contrast to the order parameter, the behavior of the central polarization depends on α . The LDA calculations, based on the conventional DMFT for homogeneous lattices at $T = 0$, show a first-order transition from the fully paired superfluid phase to the partially paired normal phase without the intermediate polarized superfluid phase. However, the LDA cannot consider the inhomogeneous exotic phase observed in Fig. 1, and it ignores the interface effects that may contribute to the polarized superfluidity. While the potential role of finite-size effects should not be ruled out, we have tested also $N \simeq 320$ and found the same features.

FIG. 2 (color online). Transition to the normal phase with increasing polarization P examined for various trap aspect ratios α . (a) Superfluid order parameter $\sum_i |\Delta_i|^2 / N_{\downarrow}$ vanishes above $P_c \simeq 0.8$, regardless of α . (b) Central polarization $(n_{\uparrow} - n_{\downarrow}) / (n_{\uparrow} + n_{\downarrow})$ of the site at the cloud center becomes finite far below P_c , implying the presence of a polarized superfluid core with finite δn and Δ as indicated in the inset. The conventional DMFT data with LDA are given for comparison.

Let us discuss in detail how the cloud structure and the pairing evolve as P increases. Figure 3 presents the axial profiles of densities $n_{\uparrow,\downarrow}$, their difference δn , and the pair potential Δ along the z axis. The data with $\alpha = 7.5$ are shown as a representative example. The fully polarized edges are well separated from the superfluid core with the partially polarized intermediate regions, while the central region shows nonuniform Δ that changes with P . Our LDA data (not shown) gives the three-shell structure: the fully paired superfluid core, partially polarized normal state shell, and fully polarized edges. This perfectly agrees with those from the QMC calculations with LDA [28]. While, at low P 's, our real-space DMFT presents a similar shell structure, the density profiles indicate the exotic superfluid phase at high P 's that is not accessible by the LDA with conventional DMFT.

At very low polarization $P = 0.08$, the core is fully paired, and small oscillations of Δ appear in the partially polarized intermediate shoulders of δn . As P increases, polarization becomes finite at the center, leading to the wide dip area with finite δn , indicating the polarized superfluid core. The dip region gets narrower with increasing P while the shoulders with small Δ oscillations get wider.

When P increases further, the dip in δn finally disappears, and the FFLO-type oscillations in Δ spread across the trap center, as plotted for $P = 0.74$ in Fig. 3. As P approaches P_c , the amplitude of Δ becomes smaller and finally vanishes at P_c . Along with the oscillating Δ , we also find the corresponding oscillations in δn with a half period of Δ . This is consistent with the prediction of the FFLO-type phase in one dimensional (1D) systems [29]. However, our systems still show 3D features: at low P 's, density profiles are similar to the LDA data in 3D while fully paired edges together with the FFLO phase at the center are expected in the strictly 1D system [17,29].

We find that these FFLO-type oscillations emerging across the trap center, rather than residing just at the edges, are found only in highly elongated traps with the trap aspect ratios $\alpha \geq 5.0$ among the examined values of α 's. The dependence of the core phase on α is summarized in Fig. 4. For $\alpha = 1.0$ and 2.5, we have found the oscillations of Δ reside only at the edges for all $P < P_c$.

The diagram in Fig. 4 separates the phases of the central region of the traps into fully paired superfluid (SF), polarized superfluid (pSF), FFLO, and normal (N). The FFLO-type phase can be signaled by the disappearance of the central dip in δn , as shown in Fig. 3. The boundary between SF and pSF is rather unclear because δn becomes finite gradually with increasing P . However, our calculations show a tendency for the central polarization to grow faster as the trap gets more elongated.

The nature of the polarized superfluidity found in our real-space DMFT calculations at $T = 0$ can be very subtle. It has not been clear yet how stable pSF is at $T = 0$, especially in a trap. The breached-pair state is in general energetically unstable toward the phase separation at a weak coupling at $T = 0$ [30,31]. For a strong coupling, an earlier DMFT calculation in half-filled homogeneous cubic lattices found that the pSF may be stable down to a very low temperature [32], while other calculations suggested that the density difference may decay exponentially with decreasing temperature in quarter-filled infinite dimensional lattices [33]. In our LDA calculations, we have observed a sharp SF-N transition without an intermediate pSF phase. The stability issue can be more complex in our trapped asymmetric systems. We have found nonstandard (pSF)-FFLO-N-type structures in the elongated traps, which cannot be explained with LDA.

Our real-space DMFT inspires the question: how different are the results qualitatively from those given by the BdG *static* mean-field theory, incorporating a trapping potential [34]? The DMFT is based on a discrete lattice system, nevertheless we choose to compare it to a BdG approach without a lattice (the density of our lattice fermions is well below the quarter filling). In Fig. 5, we observe very high P_c (~ 0.95) and the strong deformation of the core shape at high P 's. These features are in clear contrast with those found in our real-space DMFT. The DMFT accurately describes local quantum fluctuations which are missing in the BdG theory that does not properly include interactions in the normal state. Such effects cause the large deviation in P_c in the strongly interacting regime.

The explicit test for the trap aspect ratio sheds light on the comparison between the experiments [13,15] and [14].

FIG. 3 (color online). Evolution of the cloud structure with increasing polarization P . Axial density profiles n and pair potential Δ are shown along the z axis. The plots are selected for the trap aspect ratio $\alpha = 7.5$. The coexistence of the finite dip in the density difference $\delta n \equiv n_{\uparrow} - n_{\downarrow}$ and a finite Δ at the central region characterizes the polarized superfluid core. The central dip in δn disappears at high $P = 0.74$, replaced by the FFLO-type oscillations in $\Delta(z)$ spreading across the trap center.

FIG. 4 (color online). Trap aspect ratio α and polarization P dependence of the phase of the central region of the trap. Fully paired superfluid (SF) is found at low P 's and continuously evolves into the polarized superfluid (pSF). The pSF is specified with the central polarization larger than 0.005. At higher P 's, the FFLO-type phase is identified for $\alpha \geq 5.0$. The dashed lines between the phases are drawn for guidance.

Despite the difference between dilute gases and low-filling lattice fermions considered here, the critical polarization and the three-shell density profiles that we have found out are in good agreement with [13,15,16]. While the very large aspect ratio $\alpha \sim 45$ used in [14] is not accessible because of computational limitations, we have not found any signatures of changing density profiles when increasing the trap aspect ratio.

The exotic superfluid phases found in our study suggest that high polarizations $P \leq P_c$ can be an interesting area for future experiments with spin-imbalanced Fermi gases. In our calculations at $T = 0$, we have found that the FFLO-like phase emerges at high polarizations close to P_c . The amplitude of the oscillating pair potential across the trap center is expected to be still significantly large, which implies that it may be experimentally accessible at low but finite temperatures. In addition, the density and pair potential profiles that we have found in elongated traps reveal the 3D characteristics which are essentially different from the profiles predicted in strictly 1D. This emphasizes

FIG. 5 (color online). BdG calculations at unitarity in the elongated trap with $\alpha = 10$. (a) The condensate fraction is plotted as a function of polarization P . (b) The density difference δn_{BdG} and (c) the pair potential Δ_{BdG} (normalized by the Fermi energy E_F) in the $y = 0$ plane are shown for selected P 's. The majority population $N_\uparrow$ is fixed at 200 for a given P .

the possibility for the experimental observation of the FFLO phase in 3D systems.

This work was supported by the Academy of Finland (Projects No. 213362, No. 217043, No. 217045, No. 210953, No. 135000, No. 139514) and EuroQUAM/FerMix, and conducted as a part of a EURYI scheme grant (see www.esf.org/euryi). Computing resources were provided by CSC—the Finnish IT Centre for Science and the Triton cluster at the Aalto University.

*paivi.torma@hut.fi

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