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Finite-temperature stability and dimensional crossover of exotic superfluidity in lattices

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We investigate exotic paired states of spin-imbalanced Fermi gases in anisotropic lattices, tuning the dimension between one and three. We calculate the finite temperature phase diagram of the system using real-space dynamical mean-field theory in combination with the quantum Monte Carlo method. We find that regardless of the intermediate dimensions examined, the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state survives to reach about one third of the BCS critical temperature of the spin-density balanced case. We show how the gapless nature of the state found is reflected in the local spectral function. While the FFLO state is found at a wide range of polarizations at low temperatures across the dimensional crossover, with increasing temperature we find out strongly dimensionality-dependent melting characteristics of shell structures related to harmonic confinement. Moreover, we show that intermediate dimension can help to stabilize an extremely uniform finite temperature FFLO state despite the presence of harmonic confinement.

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Fermion pairing in the presence of spin-density imbalance has been a fundamental issue in many strongly correlated systems of many fields ranging from superconductors to ultracold atomic gases and neutron stars.1 While a large magnetic field is detrimental to BCS superconductivity,2,3 it has been predicted that a more exotic pairing mechanism would maintain Cooper pairs coexisting with finite spin-density imbalance. The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state suggests a promising scenario where, with spin polarization, Cooper pairs carry nonzero center-of-mass momentum, exhibiting a spatially oscillating order parameter.4,5 In three-dimensional continuum, the previous mean-field studies predicted only a tiny FFLO area in the phase diagram.6 Indeed, the FFLO state remains elusive in experiments in spite of indirect evidence of its existence reported in several fields.7–11 However, the stability of the FFLO state has been suggested to depend rather sensitively on system settings, such as the presence of lattices,12–15 the dimensionality,16–22 and the trap aspect ratio.23 In particular, it has been anticipated that the FFLO signature would be much more visible in a dimensional crossover regime between one-dimensional (1D) and three-dimensional (3D) systems where the strong 1D-FFLO character at zero temperature could be further stabilized by the long-range order supported by higher dimensions.

In this paper, we provide finite temperature phase diagrams of spin-polarized Fermi gases in lattices of intermediate dimensions in a 1D-3D crossover regime. Intermediate dimensions are accessible in ultracold atomic gases by controlling optical lattices as realized for weakly coupled 1D tubes14 and chains.24 Previous works on the FFLO state in the dimensional crossover regime are done at the mean-field level for coupled tubes15,25 or at zero temperature for two-leg ladders26 and lattices.27 However, finite temperature effects are of fundamental importance and need to be fully understood to form a precise picture on the observability of exotic paired states, especially regarding shell structures of different phases that occur because of the overall harmonic trap present in ultracold gas experiments. While at close to 1D the scaling of critical temperature was studied by the effective field theory,21 to our knowledge the finite temperature phase diagram in the intermediate dimension has not been systematically approached so far. By employing a real-space variant of dynamical mean-field theory (DMFT)23,28,29 with continuous-time auxiliary-field quantum Monte Carlo method,30–32 we explicitly consider the effects of local quantum fluctuations at finite temperatures beyond the mean-field level, and the presence of a trap potential which is essential to the shell structures.

We consider a trapped, attractively interacting two-component Fermi gas in an optical lattice of 1D chains which are coupled to form an anisotropic cubic lattice [see the inset of Fig. 1(a)]. For deep lattice potentials, this system is described by the Hubbard Hamiltonian

$$\mathcal{H} = -t \sum_{i,\sigma} (c_{i+1,\sigma}^\dagger c_{i,\sigma} + \text{H.c.}) - t_\perp \sum_{i,\sigma} \sum_{i',\sigma'} c_{i,\sigma}^\dagger c_{i',\sigma'} + U \sum_{i,\sigma} \hat{n}_{i,\sigma} \hat{n}_{i,\sigma} + \sum_{i,\sigma} (V_{i} - \mu_{\sigma}) \hat{n}_{i,\sigma}.$$ 

Here \(\sigma = \uparrow, \downarrow\) denotes the (pseudo) spin state, while \(i\) and \(l\) stand for the chain and the lattice site within the chain, respectively. The fermionic annihilation and creation operators are \(c_{i,\sigma}\) and \(c_{i,\sigma}^\dagger\), and \(\hat{n}_{i,\sigma}\) is the density operator. We consider a harmonic potential \(V_{i} = \omega_{i}^2 l^2 / 2\) along the chains. The model is parameterized by the interaction strength \(U\), the trap frequency \(\omega_{i}\), the spin-dependent chemical potential \(\mu_{\sigma}\), and the intra- and interchain hoppings \(t_1\) and \(t_\perp\), respectively. All energies and temperatures are in units of \(t_1\), and we set \(\hbar = 1\). Varying the interchain hopping \(t_\perp\) from zero to one the system undergoes a dimensional crossover from a collection of 1D chains to a 3D (cubic) lattice. In the calculations, the trap frequency is set to \(\omega_{i} = 1.1 \times 10^{-2}\). The chemical potentials are varied to control the polarization \(P = (N_{\uparrow} - N_{\downarrow})/(N_{\uparrow} + N_{\downarrow})\) while keeping the total particle number constant at \(N_{\uparrow} + N_{\downarrow} \approx 100\) per each chain. The interaction strength \(U\) is chosen for each value of \(t_\perp\) to correspond to the lattice equivalent of the unitarity limit,33 and thus, the interaction strength is fixed by

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a fundamental two-body property. A further investigation of an optimal interaction strength for the realization of the FFLO state remains beyond the present work.

In DMFT, the self-energy of the system is taken as site diagonal, i.e., $\Sigma_{i,i'}(i\omega_n) = \delta_{i,i'} \delta_{i,i'} \Sigma_{i,i'}(i\omega_n)$. We consider the system and all physical quantities to be homogeneous in the interchain direction, and therefore, the self-energy becomes independent of the chain index $i$. Thus, the Green’s function of the system can be written as

$$[G^{-1}(k_\perp;i\omega_n)]_{ij} = [G_{ij}^0(i\omega_n)]_{ij}^{-1} - [\epsilon_{k_\perp}\sigma_3 + \Sigma_{i,i'}(i\omega_n)]_{ij},$$

in which $G_{ij}^0$ is the noninteracting Green’s function of a single chain, $\omega_n$ is the Matsubara frequency, and $\sigma$ is the Pauli matrix. The transverse kinetic term is given by the dispersion $\epsilon_{k_\perp} = -2t_L (\cos k_x + \cos k_y)$ with the transverse quasimomentum $k_\perp = (k_x, k_y)$. In this notation, the bath Green’s function of the DMFT calculations is given as

$$[G_{ij}^0(i\omega_n)]_{ij}^{-1} = [\Sigma_{i,i'}(i\omega_n)]_{ij}^{-1} + \Sigma_{i,i'}(i\omega_n).$$

The pairing order is considered within the Nambu formalism, and the order parameter is defined as $\Delta_i = -\langle c_{i,\uparrow}^\dagger c_{i,\downarrow}\rangle$.

We present the phase diagrams for a quasi-1D system with $t_L = 0.2$, a system of intermediate dimensionality with $t_L = 0.4$, and a quasi-3D system with $t_L = 0.8$ in Fig. 1. The order of the phase transitions in Fig. 1 remains an open question in our study, and it is possible that the phase boundaries are crossovers because of the finite trap potential. We find that throughout the dimensional crossover, the ratio of the maximum FFLO critical temperature and the balanced BCS critical temperature is $T_{c,\text{FFLO}}^\text{c,max}/T_{c,\text{BCS}}^\text{c,max} \approx 1/3$. Taking the temperature of 0.7$T_{c,\text{FFLO}}^\text{c,max}$ as a reference point, we find that the polarization window for the FFLO phase grows gradually towards the quasi-3D limit from a value of $\delta P = 0.06$ at $t_L = 0.2$ to $\delta P = 0.10$ at $t_L = 0.8$.

In the quasi-1D regime we find a superfluid order parameter which has its maximum value away from the center of the trap; this is clearly visible in the FFLO state of Fig. 1(a). In this regime the FFLO state melts to the shell structure of the general type displayed in Fig. 1(c) in which there is a...
polarized superfluid on the edges of the trap and an oscillating order parameter at the center, labeled as cFFLO in Fig. 1(a). However, above \( P = 0.18 \) the system starting from the FFLO state reaches with increasing temperature the normal state in the middle of the trap (cN) and not the cFFLO shell structure. The maximum critical temperature of the cFFLO phase is \( T_{C,\text{max}} = 0.45 T_{C,\text{BCS}} \). Below the polarization of \( P = 0.13 \) the cFFLO shell structure melts further to a polarized superfluid phase, and above \( P = 0.13 \) to the cN shell structure with the normal state in the middle of the trap.

The phase diagrams for systems of intermediate dimensionality (\( t_{\perp} = 0.4 \)) and for quasi-3D (\( t_{\perp} = 0.8 \)) are qualitatively similar. In particular, we always find the strongest pairing in the middle of the trap similar to a 3D system. Comparing Figs. 1(e) and 1(f) we see how, here in the case of \( t_{\perp} = 0.4 \), the FFLO state melts to the polarized superfluid phase at constant polarization. It is noteworthy, that in the pSF phase the edge of the superfluid still exhibits an FFLO-type oscillating order parameter, which gradually disappears with increasing temperature. As indicated in Figs. 1(d) and 1(g), there is a transition from FFLO to the normal phase above the polarizations \( P = 0.27 \) and \( P = 0.34 \) for \( t_{\perp} = 0.4 \) and \( t_{\perp} = 0.8 \), respectively. Figures 1(h) and 1(i) demonstrate how the FFLO state responds to an increase in temperature at constant polarization; the paired region recedes towards the middle of the trap. Furthermore, the magnitude of the order parameter decreases while the wavelength of the FFLO oscillation grows; this observation holds at all dimensionalities. At the low temperature limit of the phase diagrams, we find good agreement with the zero temperature results of Ref. 27.

Throughout the crossover, the lower boundary of the FFLO region in the phase diagram with respect to polarization increases with temperature. This behavior is essentially explained by the fact that at higher temperatures, the polarized superfluid accommodates a larger spin-density imbalance within its thermal excitations. In the shell structure of a trapped gas this leads to an additional effect which counteracts the FFLO instability. Namely, the polarization can be redistributed towards the BCS-like regions with increasing temperature. On the other hand, higher temperatures are less favorable for any pairing effects to take place and thus the upper boundary of the FFLO region with respect to polarization is diminished by temperature. Consequently, throughout the crossover the highest attainable critical temperature for FFLO is rather sensitive to polarization.

Intriguingly, we find that the amplitude of the FFLO order parameter is essentially uniform, as shown in Fig. 2, in a broad polarization and temperature range at the interchain hopping of \( t_{\perp} = 0.3 \). This is also the crossing point between 1D-like and 3D-like physics. For instance at the temperature of \( T = 0.05 \), such uniform behavior occurs in a 60% interval of the FFLO polarization range in the phase diagram which is at this temperature \( \delta P = 0.09 \). This suggests that the “sweet spot” anticipated in Ref. 19 for observing the textbook FFLO order parameter resides at \( t_{\perp} \approx 0.3 \). The uniformity can also be an advantage for observing the state, considering probes that rely on strict periodicity of the order parameter.

Further characteristics of the FFLO state can be inferred from the local spectral function plotted in Fig. 3. The local spectral function is defined as \( A_{j,\sigma}(\omega) = -2 \text{Im} G_{j,\sigma}(i\omega_n) \rightarrow \omega + i0^+ \), and can be interpreted as the local density of states. We use the maximum entropy method to carry out the analytical continuation from the on-site Green’s function obtained from the QMC solver. From the spectral function one can clearly see that the FFLO state is gapless, and also in this sense the well-known mean-field characterization of the state remains valid. Moreover, we find that only the energy states very close to the Fermi level contribute to the formation of the FFLO density oscillation.

In conclusion, our work, which incorporates both finite temperature effects and local quantum fluctuations, shows that the FFLO state is significant throughout a dimensional crossover between 1D and 3D lattices at finite temperatures. The critical temperature of the FFLO state is approximately

![FIG. 2.](image-url) (Color online) At the crossing point between quasi-1D and 3D-like behavior, at \( t_{\perp} = 0.3 \) (\( U = -3.75 \)), we find that the FFLO state (here with \( P = 0.17 \) and \( T = 0.04 \)) exhibits an exceptionally uniform oscillation amplitude across the whole system in spite of a density profile varying with the trap potential.

![FIG. 3.](image-url) (Color online) (a) The FFLO state near the trap center with \( t_{\perp} = 0.8 \), \( T = 0.067 \), and \( P = 0.30 \). The local spectral functions of the FFLO state on the lattice sites b and c of panel (a) for \( \sigma = \uparrow, \downarrow \) are plotted in panels (b) and (c), respectively. The oscillation of the density profile is revealed to affect the most particles at energies close to the Fermi surface. The gapless nature of the FFLO state is clearly visible in the majority (\( \uparrow \)) component on site c, i.e., at the node of the order parameter.
one third of the superfluid critical temperature regardless of the dimensionality, reaching values as high as $T \simeq 0.13 t_f$.

We find that dimensionality has a clear effect on the melting behavior of the shell structures in a trap, which is essential in distinguishing between the different phases. Furthermore, we identify $t_L = 0.3$ as the dimensionality crossover point that provides the sweet spot of observing a uniform FFLO order parameter despite the harmonic trap confinement. On a final note, our results confirm that, even at the presence of local quantum fluctuations, the FFLO state has a wide region of stability in a lattice, which is in stark contrast to the theoretical predictions in free space where the parameter area for the FFLO state is vanishingly small. This gives evidence to the fundamental role the Fermi surface shape has in stabilizing exotic superfluidity, and brings about a significant degree of freedom to future experiments aimed to realize elusive phases of matter such as the FFLO state. From the theoretical point of view it remains an important problem to quantify whether *nonlocal* quantum fluctuations play a significant role in the physics of the dimensional crossover and the FFLO state.

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