Interplay between exotic superfluidity and magnetism in a chain of four-component ultracold atoms

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We investigate the spin-polarized chain of ultracold alkaline-earth-metal atoms with spin-3/2 described by the fermionic Hubbard model with SU(4) symmetric attractive interaction. The competition of bound pairs, trions, quartets, and unbound atoms is studied analytically and by density-matrix renormalization-group simulations. We find several distinct states where bound particles coexist with the ferromagnetic state of unpaired fermions. In particular, an exotic inhomogeneous Fulde-Ferrell-Larkin-Ovchinnikov (FFLO)-type superfluid of quartets in a magnetic background of uncorrelated atoms is found for weaker interactions. We show that the system can be driven from this quartet-FFLO state to a molecular state of localized quartets where spatial segregation between molecular crystals and ferromagnetic liquids emerges, and this transition is reflected in the static structure factor.

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I. INTRODUCTION

Investigating effective Hamiltonians with local contact interactions has proven to be instrumental in understanding the physics of ultracold atomic systems [1–3]. Realizing exotic quantum states, e.g., inhomogeneous Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superfluid pairs [4,5] or trionic states [6], low-dimensional systems are of particular interest owing to the large quantum fluctuations [7–16]. Thanks to rapid progress in the experimental techniques in the physics of ultracold atoms, by now not only two-component systems can be experimentally realized but an insight into unconventional molecular superfluids of multiple-body states is also provided [11,17–32], which urges further studies of the detailed properties of such systems.

The phase diagram of the one-dimensional four-component interacting Fermi gas with s-wave scattering is well established. It exhibits various exotic superfluid phases, among them a phase with SU(4)-singlet quartets [28,33–39]. Contrary to this, the behavior in an external magnetic field where a finite spin imbalance develops is still an open question. For attractive interactions far detuned from SU(4) symmetry, we observed a mixing of spin-carrying pairs and spin-neutral quartets in our earlier work [40,41]. In the case of experimentally more relevant SU(4) symmetric couplings it is expected that the quartets are replaced at least partially by other energetically favorable spin-carrying excitations [10].

In this paper, we study the competition between magnetism and superfluidity in the SU(4) symmetric Hubbard-like four-component model in external magnetic field B,

$$\mathcal{H} = -t\sum_{i,\alpha}^{L}(\hat{c}^{\dagger}_{\alpha,i}\hat{c}_{\alpha,i+1} + \text{H.c.}) + \frac{U}{2}\sum_{i=1}^{L}\hat{n}_i^2 + pNB, \quad (1)$$

by controlling the spin imbalance p. Here, L is the length of the chain and operator $\hat{c}^{\dagger}_{\alpha,i}$ creates a fermion with spin $\alpha \in \{-3/2,-1/2,1/2,3/2\}$ at site i. The number operator reads $\hat{n}_i = \sum_\alpha \hat{n}_{\alpha,i}$ and $p = \frac{1}{L}\sum_{i,\alpha}\alpha\langle\hat{n}_{\alpha,i}\rangle$. The total number of particles is N, t measures the one-particle overlap between neighboring sites, and $U < 0$ parametrizes the strength of the SU(4) symmetric attraction between alkaline-earth-metal atoms.

The quarter-filled, $N = L$, phase diagram is summarized in Fig. 1 as a function of the coupling U and polarization p. The partially polarized system exhibits three quartetting phases with strikingly distinct character for increasing $|U|$ in the four-component region. Above a critical polarization only $\alpha > 0$ fermions are present in the system; i.e., we observe a gapless two-component liquid. We found that a three-component system emerges for weak or intermediate interactions, while a direct transition between phases with four and two fermion components is observed in the case of strong enough couplings. In what follows we first give a qualitative description of the behavior of the model in the bosonization representation and then we present the results of numerical calculations using the density-matrix renormalization-group (DMRG) method [42,43].

II. BOSONIZATION

The properties determined by low-energy excitations can be well understood within a hydrodynamical treatment taking into account only those states which are in the vicinity of the Fermi energy. In the case of spin balance the populations of the four spin states are equal, and there are only two Fermi points, $\pm k_F$.

Switching on spin imbalance this degeneracy is removed and the Fermi momenta shift, leading to eight different Fermi points at $\pm k_\alpha$'s. Using standard notation [44,45], in boson representation the total Hamiltonian can be written in the

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form

$$H = \frac{1}{\pi}\sum_{\alpha}\int dx\left\{\left(2v_\alpha + \frac{U}{\pi}\right)(\partial_x\phi_\alpha)^2 + 2v_\alpha(\partial_x\theta_\alpha)^2 + \frac{U}{\pi}\sum_{\alpha'(\neq\alpha)}\partial_x\phi_\alpha\partial_x\phi_{\alpha'} + \lambda_\alpha\partial_x\phi_\alpha + \frac{U}{2\pi}\sum_{\alpha'}\cos[2(\phi_\alpha - \phi_{\alpha'})] + g_u\sum_{\alpha'}\cos\left[2\sum_{\alpha}\phi_\alpha\right]\right\}, \tag{2}$$

where the Gaussian part describes the small momentum transfer scattering processes, while the cosine terms describe the ones with large momentum transfer. g_u drives the four-particle umklapp processes which may appear at quarter filling and g_u is proportional to U^3. We introduce a spin-dependent Lagrange multiplier λ_α to fix the global occupation number of the spin components and the total particle number per site. The constraints on filling and polarization can be ensured with two independent Lagrange multipliers λ_n and λ_s with $\lambda_\alpha = \lambda_n + \alpha\lambda_s$. With this the explicit expression of the shifted Fermi momenta is $k_\alpha = k_\mathrm{F} + \mu_\mathrm{B}\alpha\lambda_s$, where μ_B is the Bohr magneton, and $\alpha = \pm 1/2, \pm 3/2$. After the diagonalization of the Gaussian part of Hamiltonian (2) in the spin space, the linear term $\lambda_\alpha\partial_x\phi_\alpha$ can be transformed out by a simple shift of the new bosonic fields.

When the interaction is weak compared to the energy contribution of the magnetization and only particles close to the Fermi points can be excited and can participate in scattering processes, the quasimomentum conservation cannot be satisfied by these relevant particles in the large-momentum-transfer scattering processes [44]. This means that the spin imbalance freezes out the real backscatterings and one arrives at a Gaussian problem. In the case of quarter filling, similarly to the backward scatterings, the four-particle umklapp processes are also frozen out for weak interactions. In this case all bosonic fields ϕ and their duals θ can fluctuate freely, and the dominant instability is a $2k_\mathrm{F}$ density order ($O_{2k_\mathrm{F}} \propto e^{i2\phi_\alpha}$) with subdominant pairing, trioning, and quartetting. Further increase of the spin polarization freezes out the spin components one by one, and the system becomes equivalent to a three- and a two-component system, respectively. In principle, these transitions are not necessarily simple; i.e., close to the transition points a finite spin gap could be expected to pin the density fluctuations, whenever the backward scatterings become sufficiently strong as we discussed above. However, we see that our numerical results predict that the system stays in the Gaussian state even close to the transition lines. In Fig. 1 this phase is referred to as a Gaussian (Luttinger) liquid with different color for the different number of the spin component n. Upon further increasing the polarization, it obviously saturates at $p = 3/2$, and a liquid state of unbound fermions with maximum spin projection ($\alpha = 3/2$) is stabilized. This trivial, $n = 1$, fully polarized phase is not indicated in Fig. 1.

As a consequence of the spin imbalance, the chargelike mode does not correspond to the symmetric combination of the density of the spin components $n_\mathrm{tot} = \sum_\alpha n_\alpha$, but a weighted sum of them: $n^\mathrm{w}_\mathrm{tot} = \sum_\alpha a_\alpha n_\alpha$ with $a_\alpha = \sqrt{\frac{\sin(k_\alpha)}{\sin(\pi/4)}}$. Introducing

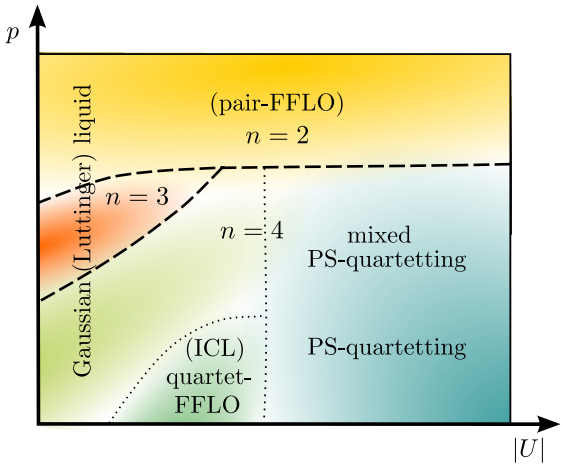

FIG. 1. Schematic phase diagram of spin-3/2 fermionic atoms as a function of the attractive spin-independent interaction strength $|U|$ and the polarization $0 < p < 3/2$. The dashed lines indicate transitions between phases consisting of different numbers of spin components $n = 2$, 3, and 4. The $n = 1$ fully polarized phase is not indicated. The lines are only a guide to the eyes.

the new fields $\phi_\alpha \to a_\alpha\phi_\alpha$ the threefold-degenerate eigenvalue of the Gaussian part of Hamiltonian (2) corresponds to the spinlike modes, while the nondegenerate eigenvalue gives the ratio of the sound velocity and the Luttinger parameter of the chargelike mode u_c/K_c. Figure 2 shows the characteristic behavior of the four eigenvalues, and the Luttinger parameter K_c. We find that K_c becomes divergent at a critical interaction strength determined by the equation $u_c/K_c = 0$. However, the compressibility is directly related to n_tot; the above singularity in the Luttinger parameter of the chargelike weighted mode also indicates density instability and the possibility of phase separation in the system for stronger interactions—beyond the validity of the hydrodynamical picture. This first-order transition is supported by strong numerical evidences (see below) and indicated in Fig. 1 by a dotted line between the Gaussian liquid of the four-component system and the phase-separated (PS) quartetting phase.

In the case of intermediate couplings one has to deal with the backscatterings, and the four-particle umklapp processes, too. Due to the different occupations of the four spin components, all bosonic fields are coupled by the cosine terms in Eq. (2). Accordingly, relevant processes can open both the charge and

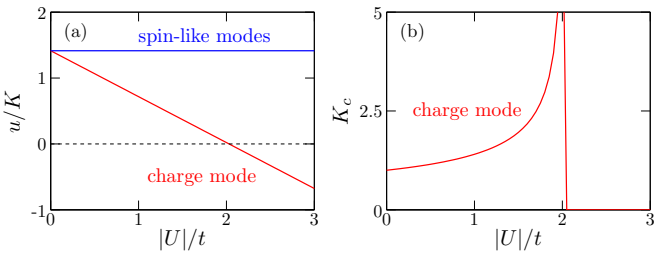

FIG. 2. (a) Eigenvalues of the Gaussian part of Hamiltonian (2) as a function of the coupling U, and (b) the divergence of the Luttinger parameter of the charge mode K_c indicating the density instability which leads to phase separation in the system.

the spin gap, leading to an incompressible liquid (ICL) state. In this case only the dual fields θ fluctuate freely; therefore, the competing correlations are the tunneling density $O_G \propto e^{i2\theta_\alpha}$, and the various composite states: pairing $O_P \propto e^{i2(\theta_\alpha+\theta_{\alpha'})}$, trioning $O_T \propto e^{i2(\theta_{\alpha_1}+\theta_{\alpha_2}+\theta_{\alpha_3})}$, and quartetting $O_Q \propto e^{i2\sum_\alpha \theta_\alpha}$. However, the tunneling density shows always the slowest decay; the system can be characterized by the off-diagonal orders of the competing composite bound states. For weak spin imbalance, the interaction is sufficiently strong to suppress the magnetic energy. In this regime our numerical analysis supports that the system is indeed a gapped incompressible liquid. The corresponding phase is indicated in Fig. 1 as quartet-FFLO (ICL), notation that is based on the details of our numerical findings discussed below.

III. NUMERICAL RESULTS

In order to establish a complete phase diagram of the system we performed numerical calculations using the DMRG method with open boundary condition up to $L = 72$ sites. The accuracy was controlled by the dynamic block state selection (DBSS) procedure [46,47], keeping up to 2000 block states and performing 8 sweeps. In addition to the various correlation functions and their Fourier transforms, we study local densities measuring the exclusive occupation number of unbound atoms and various molecules composed of two, three, or four fermions. As examples, the explicit formula for $\alpha = 3/2$ free atom, quintet pair with $m = 2$, trion with $\alpha = 3/2$, and quartet read

$$\begin{aligned} A_{3/2,i} &= \langle(1-\hat{n}_{-3/2,i})(1-\hat{n}_{-1/2,i})(1-\hat{n}_{1/2,i})\hat{n}_{3/2,i}\rangle, \\ P_{2,2,i} &= \langle(1-\hat{n}_{-3/2,i})(1-\hat{n}_{-1/2,i})\hat{n}_{1/2,i}\hat{n}_{3/2,i}\rangle, \\ T_{3/2,i} &= \langle(1-\hat{n}_{-3/2,i})\hat{n}_{-1/2,i}\hat{n}_{1/2,i}\hat{n}_{3/2,i}\rangle, \\ Q_i &= \langle\hat{n}_{-3/2,i}\hat{n}_{-1/2,i}\hat{n}_{1/2,i}\hat{n}_{3/2,i}\rangle, \end{aligned} \tag{3}$$

respectively. Results presented in the following are based on detailed calculations for $U/t \in \{-0.1,-0.5,-1,-2,-3,-4,-8,-20,-50,-100\}$.

Starting from the unpolarized case ($p = 0$) our numerical study confirms the earlier results [28,34,35,37] about the gapless Gaussian state in the very weak interaction regime ($|U|/t \leqslant 1$), and the formation of quartets for moderate attractive interactions ($1 < |U|/t \leqslant 50$). For extremely strong interactions ($|U|/t = 100$)—far beyond the validity of the field-theoretical description—we found that the quartets show a tendency to become localized as the effective repulsion between neighboring quartets, $\sim t^2/|U|$, overwhelms their effective hopping amplitude, $\sim t^4/|U|^3$. In our numerical investigation, the highly degenerate crystals compete energetically with the gapped liquid state observed for weaker interactions. Given the extremely small energy scale needed to be resolved, the ground state cannot be unambiguously determined via numerics.

Polarizing the weakly interacting system up to moderate values, the ground state does not change drastically compared to the spin-balanced case. The correlation functions still show power-law decay, and the system remains in the Gaussian state as the phase diagram in Fig. 1 shows. However, as the polarization is increased, the weight of the $m = 2$ pairs formed of $\alpha = 3/2$ and $1/2$ fermions increases and their correlations become dominant over quartet decay. For sufficiently large polarizations, where the gapless system contains exclusively $\alpha > 0$ particles and is therefore half filled, the Green's function of the majority component ($\alpha = 3/2$) is dominant. Nevertheless, the slow algebraic decay of $m = 2$ pair correlations with spatial oscillation periodicity proportional to the population imbalance can be interpreted as FFLO pairing [48] (also depicted in Fig. 1).

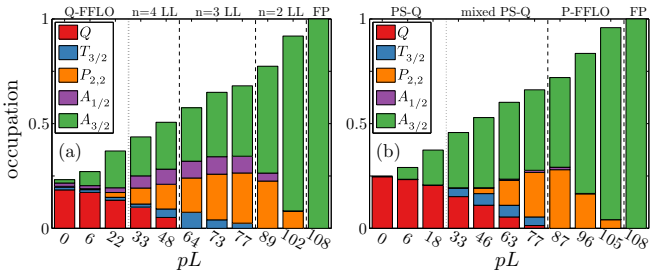

FIG. 3. (a) Average occupation number of the characteristic composite particles in the chain with $L = 72$ sites measured in representative p values for $U/t = -2$. (b) Similar for $U/t = -8$.

For intermediate attractive interactions ($|U|/t \in \{2,3\}$), where quartetting becomes more prominent, the SU(4)-singlet quartets of the unpolarized ground state start to dissolve into a mixture with $\alpha = 3/2$ unpaired fermions as the spin balance is broken (see Fig. 3). The nature of the quartets can be caught by the analysis of their center of mass (c.m.) momentum distribution. An exotic FFLO-like state is found since the peak of the distribution shifts linearly with increasing polarization [49]. This quartet-FFLO state corresponds to the incompressible liquid state of the bosonization predictions as it is shown in Fig. 1. Note that in this state trions and $m = 2$ quintet pairs are also observed with small weight as shown in Fig. 3(a) for smaller values of p. As the polarization is further increased all the correlation functions start to show algebraic decay and the system becomes four-component Gaussian (see Fig. 1). Now again we found that the polarization does not affect the correlation functions in the Gaussian state, and up to intermediate couplings the spin components are frozen out one by one.

Turning now to the strongly interacting regime ($|U|/t \geqslant 4$), we observe that in the polarized system the quartet crystallization appears for significantly weaker U compared to case $p = 0$. This can be understood as follows. The spin-balanced ground state is purely characterized by quartets and their localization is owed to the strong effective repulsion as discussed above. Contrary to this, in the case of spin imbalance, the crystallization and the spatial segregation of the emerging composite particles are governed by their mass imbalance similarly to two-component systems with asymmetric hoppings [50–52]. In the present model, the asymmetry can be understood in terms of the perturbation theory: the effective hopping for pairs, trions, and quartets is of order $t^2/|U|$, $t^3/|U|^2$, and $t^4/|U|^3$, respectively [37].

In particular, for weak spin imbalance (PS quartetting in Fig. 1), quartets become crystallized and segregate from the sea of unbound $\alpha = 3/2$ atoms according to the density profiles [see Fig. 4(a)]. The c.m. of the quartets remains zero independently of p and they behave like well-localized hard-core bosons. For larger polarization, besides the free

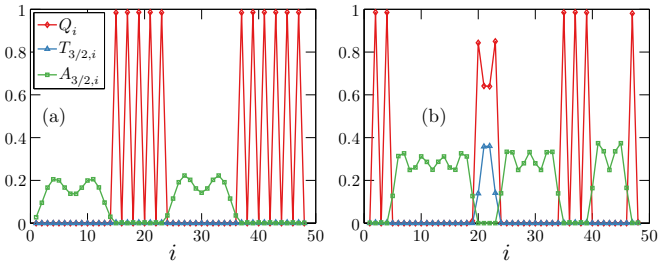

FIG. 4. (a) Typical density profile of the characteristic composite particles measured in the PS-quartetting phase ($U/t = -8$, $p = 1/8$). (b) Similar to (a) in the mixed PS-quartetting phase ($U/t = -8$, $p = 5/16$). Here, for better visibility, we present the results for a chain of length $L = 48$. The lines are only a guide to the eyes.

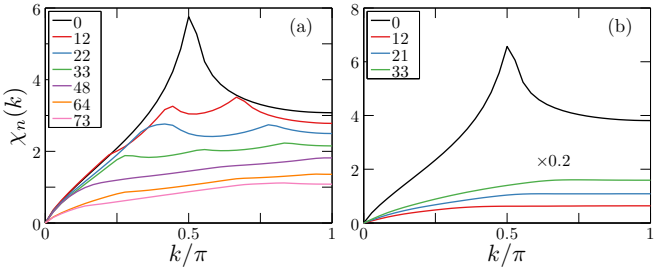

FIG. 5. (a) Fourier transform of the density correlations for $U/t = -2$ at various total imbalances $S_z = pL$, denoted with distinct colors. (b) Similar to (a) for $U/t = -8$, amplitudes for $S_z \neq 0$ are magnified by a factor of 5 for better visibility.

atoms, $\alpha = 3/2$ trions appear gradually as well. The heavy particles form domains so that the mobile $\alpha = 3/2$ fermions gain extra kinetic energy by maximized expansion [see Fig. 4(b)]. For sufficiently strong couplings, not only trions but the emerging $m = 2$ quintet pairs also become localized in the domains of the quartets. We refer to this phase as mixed PS quartetting in Fig. 1, although no sharp transition separates it from the PS-quartetting phase.

In this strong-coupling region, contrary to results for weaker interactions, the weights of the spin components $\alpha = -1/2$ and $-3/2$ vanish simultaneously as the polarization is increased [see Fig. 3(b)], implying a direct transition between the four- and two-component states. The two-component system, found for sufficiently large p, is gapless and can be characterized by the spatially nonuniform $m = 2$ pairing similarly to results for weaker couplings as depicted in Fig. 1.

IV. OBSERVABLES

The structure of the density can be probed by light-scattering diffraction measurements revealing essentially the Fourier spectrum of the density-density correlations, $\chi_n(k) = 1/L \sum_{l,l'} e^{ik(l-l')} \langle \hat{n}_l \hat{n}_{l'} \rangle$. In the case of spin balance, corroborating previous numerical analysis [35], we find that the oscillation of density correlations develops a quasicoherent peak at $\pi/2$ [see the $p = 0$ curves in Figs. 5(a) and 5(b)]. The characteristic periodicity of the density oscillations, i.e., the position of the quasicoherent peak, is determined by the Fermi momentum. For finite p, the low-energy spectrum of the system splits up and the Fermi momenta shift, leading to eight different Fermi points as was discussed in the bosonization section. As a consequence, multiple peaks emerge according to the relative population of the four spin components which can be observed nicely in Fig. 5(a).

The asymptotic behavior of the density correlations reveals the Luttinger parameter (K_c), which is proportional to the compressibility. It can be extracted from the structure factor in the long-wavelength limit, i.e., $K_c = \pi/4 \lim_{k\to 0} \chi_n(k)/k$. We observe that the Luttinger parameter of the weakly interacting system is independent of the spin imbalance up to critical polarization $p_c \approx 5/6$ where fermion component $\alpha = -3/2$ freezes out. At p_c, reaching the $n = 3$ Luttinger liquid phase with strongly asymmetrical filling, the compressibility of the system drops suddenly to a smaller value as observed in the $k \to 0$ limit of the curves in Fig. 5(a). The value of p_c does not show significant systematic changes for shorter chains either.

The phase separation can also be detected in the changing of K_c, i.e., the long-wavelength gradient of the density correlations. We found that K_c is an order of magnitude smaller in the strongly interacting spin-polarized system—even for small polarization—compared to the case of spin balance as a direct consequence of the quartet crystallization. Furthermore, the Luttinger parameter—and therefore κ also—increases slightly for increasing p as a consequence of the decreasing presence of crystallized quartet domains, and larger weight of the free atoms in the system.

V. CONCLUDING REMARKS

We investigated the phase diagram of a quarter-filled attractive four-component fermionic chain in the presence of spin polarization. We show that the system is unstable against quartet formation in the whole four-component region, but the nature of the ground state in the various phases shows fundamental differences like molecular crystallization, FFLO-like quartetting without superfluidity (gapless state), or quartet-FFLO superfluidity (gapped state). We also show that the sudden localization of the molecular quartets for stronger interactions leaves a clear fingerprint in the static structure factor.

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