Luttinger Liquid of Trimers in Fermi Gases with Unequal Masses

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We investigate one dimensional attractive Fermi gases in spin-dependent optical lattices. We show that three-body bound states—"trimers"—exist as soon as the two tunneling rates are different. We calculate the binding energy and the effective mass of a single trimer. We then show numerically that for finite and commensurate densities $n_{\uparrow} = n_{\downarrow}/2$ an energy gap appears, implying that the gas is a one-component Luttinger liquid of trimers with suppressed superfluid correlations. The boundaries of this novel phase are given. We discuss experimental situations to test our predictions.

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Recent advances with ultracold atoms are opening new prospects to address fundamental theoretical issues in direct experiments [1]. A long standing problem is whether superconductivity can coexist with the presence of an unequal number of up and down fermions. An intriguing possibility is the celebrated Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state [2], where the superconducting order parameter becomes modulated in space. The experimental search for polarized superfluids in atomic quantum gases has so far been restricted to 3D configurations [3,4]. A new and promising direction is to confine atoms in highly elongated traps, where the FFLO state is known to be very robust [5–7], as confirmed by detailed numerical simulations [8].

Another exciting topic that is currently being explored experimentally is the pairing in Fermi gases with unequal masses, like mixtures of ⁶Li and ⁴⁰K near a heteronuclear Feshbach resonance [9–11]. Alternatively, one can also trap a two-component Fermi gas in a spin-dependent optical lattice so that the corresponding effective masses are different [12]. Assuming that the transverse motion of atoms is frozen by a strong radial confinement, the system can then be described by the 1D asymmetric Fermi-Hubbard [13–15] model:

$$H_{\rm aH} = -\sum_{\langle ij\rangle\sigma} t_{\sigma} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + {\rm H.c.}) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \quad (1)$$

where U < 0 is the on-site attraction and t_{σ} are the spin-dependent tunneling rates. Here $c_{i\sigma}$ annihilates a fermion with spin σ at site i and $\hat{n}_{i\sigma}$ is the local density.

For $t_{\downarrow} = 0$ Eq. (1) is a spinless version of the Falicov-Kimball model [16], originally devised to explain metal-insulator transition in mixed-valence materials, and the corresponding ground state is known to feature a devil's staircase structure [17]. The model (1) has been recently suggested to feature Bose-Einstein condensation of d-f excitons with macroscopic polarization [18] and a spontaneous ferroelectric state [19].

For equal masses, $t_{\downarrow} = t_{\uparrow}$, the exact (Bethe ansatz) solution shows that *n*-body bound states with n > 2 are generally forbidden [20]. When the tunneling rates are

different, $t_{\downarrow} < t_{\uparrow}$, the above model is no longer integrable and many interesting questions arise: are three-body bound states (trimers) allowed? What are their properties? Can trimers open an energy gap like pairs do? And if so, what are the differences between the two gapped phases? The purpose of this Letter is to provide an explicit answer to these relevant questions. We show that there is formation of three-body bound states of two heavy (1) fermions and one light (†) fermion. We first find the regime where these trimers are stable as a function of mass asymmetry and attraction strength by solving the three-body problem. We then use the density matrix renormalization group (DMRG) method to show that at low but finite density there exists a novel phase with a nonzero energy gap which is a one-component Luttinger liquid of trimers, with exponentially suppressed superconducting FFLO correlations. Finally, we calculate the boundaries of the trimer phase in the grand canonical phase diagram. These results are in agreement with the generic bosonization analysis of Ref. [21] where the role of higher harmonics of the density operator was elucidated. The trimers discussed here are a cold atom analog of the trions recently observed in semiconductors [22]. Three-body bound states (though of different origin) have also been predicted to occur in threecomponent Fermi gases [23]. In the following we set $t_{\uparrow} = 1$ and assume $t_1 \le 1$ without loss of generality.

Three-body problem.—We start by calculating the binding energy and the effective mass of the trimer. The Schrödinger equation can be conveniently rewritten in integral form by using Green functions. For the three-body problem in a lattice one finds [24]:

$$f(k) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \frac{Uf(q)}{R_E(k)R_E(q)[\mathcal{E}(k, q) - E]},$$
 (2)

where $\mathcal{E}(k,q) = \epsilon_{\downarrow}(k) + \epsilon_{\downarrow}(q) + \epsilon_{\uparrow}(P-k-q)$, P being the quasimomentum of the trimer and $\epsilon_{\sigma}(k) = 2t_{\sigma}(1-\cos k)$ the energy dispersions of the two components. Moreover $R_E(q) = [1 + UI_E(q)]^{1/2}$, with

$$I_E(k) = \int \frac{dp}{2\pi} \frac{1}{\mathcal{E}(k, p) - E}.$$
 (3)

Equation (2) can be considered as an eigenvalue problem $\mathbf{K}_E \cdot \mathbf{f} = \lambda \mathbf{f}$, where the energy E is fixed by the constraint $\lambda = 1$. We solve this equation numerically for zero quasimomentum P = 0. The binding energy E_{tr}^b of the trimer is related to the total energy E by $-E=E_{\mathrm{pair}}^b+E_{\mathrm{tr}}^b,$ where $E_{\text{pair}}^b = -2(1+t_{\downarrow}) + \sqrt{U^2 + 4(1+t_{\downarrow})^2}$ is the binding energy of the constituent pair [25]. In Fig. 1 we plot the binding energy of the trimer as a function of the mass asymmetry t_1 for increasing values of the attraction U. We see that $E_{\rm tr}^b$ vanishes at the symmetric point $t_{\downarrow}=1$, in agreement with the Bethe ansatz solution [20]. As the mass asymmetry increases the binding energy also increases until it saturates at $t_1 \rightarrow 0$. In this limit the function (3) reduces to a constant $I_E(k) = 1/\sqrt{E(E-4)}$, implying that Eq. (2) has solution of the form $f(k) = \sin k$. Substituting this into Eq. (2) and integrating over momentum we find $E = -U^2/(1-U)$. This gives

$$E_{\rm tr}^b(t_{\downarrow} = 0) = \frac{U^2}{1 - U} + 2 - \sqrt{U^2 + 4},$$
 (4)

in agreement with our numerical solution. In particular, for infinitely strong attraction, Eq. (4) yields $E_{\rm tr}^b=1$, showing that the trimer binding energy remains finite in contrast with the pair binding energy which is instead divergent. Indeed, when the heavy particles are at neighboring sites, the light fermion can hop from one site to the other without changing the interaction energy. Therefore the total energy gain is at most equal to t_{\uparrow} . In the strong coupling limit, $|U|\gg 1$, Eq. (2) can be solved by the ansatz $f(k)=\sin k/R_E(k)$ yielding $E_{\rm tr}^b(U=-\infty)=(t_{\downarrow}-1)^2$, which is shown in Fig. 1 with black line.

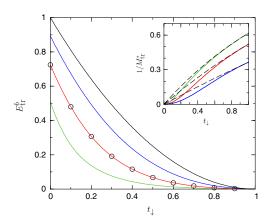


FIG. 1 (color online). Solid lines: Binding energy $E^b_{\rm tr}$ of a trimer (one light and two heavy fermions) as a function of the hopping ratio t_1 for increasing values of the attraction strength U=-2 (bottom), -4, -8, $-\infty$ calculated from the exact solution of the three-body problem. Open circles represent DMRG calculations in a chain of L=100 sites. Inset: Inverse effective mass of the trimer as a function of the hopping ratio t_1 for increasing values of the attraction strength U=-2 (top), -4, -8 shown by solid lines. At the symmetric point $t_1=1$ the bound state disappears and the effective mass reduces to the sum of the masses of constituents (dashed lines).

Let us now briefly discuss the effective mass $M_{\rm tr}^*$ of the trimer which is defined by $1/M_{\rm tr}^* = \partial^2 E/\partial P^2$ evaluated at P=0. The inverse effective mass is plotted in the inset of Fig. 1 as a function of the hopping rate t_{\downarrow} and for different values of the attraction strength. We see that the trimer becomes heavier as t_{\downarrow} decreases or |U| increases. At the breaking point, $t_{\downarrow}=1$, the effective mass reduces to $(\sqrt{4(t_{\downarrow}+1)^2+U^2}+2)/4t_{\downarrow}$, corresponding to the sum of the masses of a pair [25], and of a heavy fermion. This quantity is plotted in the inset of Fig. 1 with dashed lines.

Trimer gap.—We now turn our attention to the effects of trimers at finite density. We first calculate the trimer gap, namely, the energy needed to break a single trimer. This is defined as

$$\Delta_{\text{tr}} = -\lim_{L \to \infty} [E_L(N_{\uparrow} + 1, N_{\downarrow} + 2) + E_L(N_{\uparrow}, N_{\downarrow}) - E_L(N_{\uparrow} + 1, N_{\downarrow} + 1) - E_L(N_{\uparrow}, N_{\downarrow} + 1)], \quad (5)$$

where $E_L(N_{\uparrow}, N_{\downarrow})$ is the ground state energy of a gas with spin populations N_{\uparrow} , N_{\downarrow} in a chain of size L. The limit in Eq. (5) is taken assuming $N_{\sigma} \rightarrow \infty$ with $n_{\sigma} \equiv N_{\sigma}/L$ being fixed. The trimer gap (5) is the generalization of the binding energy at finite density, with the reference state being the many-body state $(N_{\uparrow}, N_{\downarrow})$ rather than the vacuum (0, 0). We evaluate Eq. (5) numerically via DMRG technique on lattices of up to L=160 sites with open boundary conditions and perform careful finite-size scaling in order to extract the thermodynamic limit behavior. For equal masses, $t_{\downarrow}=1$, our results are consistent with $\Delta_{\rm tr}=0$ for any concentration. For unequal masses, corresponding to $t_{\downarrow} \neq 1$, the trimer gap (5) is finite only when the two concentrations are commensurate, namely $n_{\downarrow}=2n_{\uparrow}$.

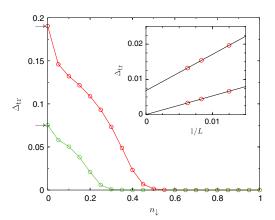


FIG. 2 (color online). Trimer energy gap plotted versus density n_{\downarrow} of the heavy component $(n_{\uparrow}=n_{\downarrow}/2)$ and for different values of the attraction U=-2 (bottom) and U=-4. The mass anisotropy is $t_{\downarrow}=0.3$. The gap $\Delta_{\rm tr}$ reduces to the binding energy $E_{\rm tr}^b$ at zero density (see arrows) and vanishes at a critical value of the density. The data are obtained from finite-size scaling after DMRG simulations with system sizes L=80, 120, 160, assuming a linear dependence in 1/L. In the inset we show the scaling analysis for two different concentrations $n_{\downarrow}=0.45$ and $n_{\downarrow}=0.6$ with U=-4.

Figure 2 shows typical results for Δ_{tr} at fixed $t_{\downarrow} = 0.3$ and $n_{\downarrow}/n_{\uparrow} = 2$. For vanishing density the trimer gap reduces to the binding energy E_{tr}^b , shown in Fig. 2 by arrows. As the density increases, Δ_{tr} decreases and eventually vanishes at a critical concentration $n_{\downarrow} = n_{\downarrow}^{cr}$ —in a sharp contrast with the case of equal densities, $n_{\uparrow} = n_{\downarrow}$, where the associated pairing gap is always positive for any filling. In other words, the opening of the trimer gap is a nonperturbative effect requiring finite coupling strength, or equivalently, low enough densities. This is consistent with our bosonization approach [21].

Correlation functions.—The opening of the trimer gap drastically affects the ground state properties of the gas, since correlation functions of all operators breaking trimers fall off exponentially rather than algebraically. In particular, the superconducting correlations decay as

$$\langle c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{j\downarrow} c_{j\uparrow} \rangle \propto \frac{\exp(-|i-j|/\xi)}{|i-j|^{\alpha}} \cos(Q|i-j|), \quad (6)$$

where the decay length $\xi \propto \Delta_{\rm tr}^{-1}$, $Q \equiv |k_F^{\uparrow} - k_F^{\downarrow}|$ is the FFLO momentum, and α is a nonuniversal number. Two-point correlations $\langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle$ display similar behavior. In Fig. 3 we explicitly check this prediction by showing the superconducting correlations in the gapped $(n_{\downarrow} < n_{\downarrow}^{\rm cr})$ and gapless $(n_{\downarrow} > n_{\downarrow}^{\rm cr})$ phases. We see that in the gapped phase the typical FFLO modulation is preserved, as discussed in Refs. [14,15], but quasi–long-range order is lost.

Phase diagram.—The presence of trimers and other bound states induced by the mass asymmetry changes the topology of the grand canonical phase diagram of the gas. The latter is obtained by replacing the densities n_{\uparrow} , \downarrow by two new variables, corresponding to the mean chemical potential $\mu = \partial E/\partial(N_{\uparrow} + N_{\downarrow})$ and the effective magnetic field $h = \partial E/\partial(N_{\uparrow} - N_{\downarrow})$, where E is the ground state energy. The evolution of the overall shape of the phase diagram

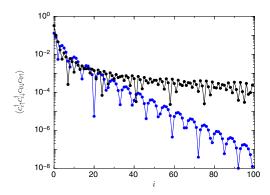


FIG. 3 (color online). Superconducting correlations as a function of the distance from the center of the chain. The upper curve corresponds to $n_{\downarrow}=0.7$, where the trimer gap is zero, cf. Fig. 2. The lower curve refers to low density $n_{\downarrow}=0.3$, where $\Delta_{\rm tr}>0$. The parameters used are U=-4, $t_{\downarrow}=0.3$, and L=200 and the densities are commensurate, $n_{\uparrow}=n_{\downarrow}/2$. Notice the change from algebraic decay (upper curve) to exponential decay (lower curve).

with changing t_1 has been presented in Ref. [15]. Here we concentrate on the nontrivial changes due to the extra bound states induced by the mass asymmetry, which were not discussed previously. To that end we work at fixed values of U and t_1 . We approximate the derivatives by finite-difference formulas similar to Eq. (5), and obtain the phase diagram shown in Fig. 4. The partially polarized phase (PP) corresponds to configurations with imbalanced spin populations $(1 > n_{\downarrow} > n_{\uparrow} > 0)$. This phase is limited from the right by the phase of equal densities (ED) $(n_{\downarrow} =$ n_1) and from below by the fully polarized (FP) phase where the minority component is absent $(n_{\uparrow} = 0)$ [26]. For equal masses, $t_1 = 1$ the three phases meet at a single point. In presence of *n*-body bound states with n > 2 this special point splits into an extended line, corresponding to a direct boundary between PP phase and vacuum. To see this, suppose there exists a bound state made of $p \uparrow$ fermions and $q \downarrow$ fermions, where p and q are non-negative integers. Since the system density is zero, the Taylor expansion $E_{L=\infty}(p,q) = (p+q)\mu + (p-q)h$ becomes yielding a straight line in the (h, μ) plane associated to the bound state. The true phase boundary $\mu = \mu_{\text{vac}}(h)$ with the vacuum is given by

$$\mu_{\text{vac}} = \min_{p,q} \frac{E_{L=\infty}(p,q) - (p-q)h}{p+q},$$
(7)

resulting in a piecewise straight line, cf. Fig. 4. While for equal masses the only states entering (7) are a single \downarrow -fermion and a pair (p=0, q=1 and p=q=1, respectively), for $t_{\downarrow} \neq 1$ additional bound states appear, e.g., trimers (p=1, q=2), quadrimers (p=1, q=3), etc.—leading to an extended PP-vacuum boundary, as shown in

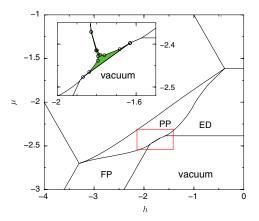


FIG. 4 (color online). Phase diagram for unequal masses obtained from DMRG simulations. Here $t_{\downarrow}=0.3$ and U=-4. The novel line boundary between partially polarized phase and vacuum is a consequence of the existence of n-body bound states with n>2. Inset: a zoom-in of the low density region of the PP phase. The locus of commensurate densities $n_{\uparrow}=n_{\downarrow}/2$ corresponds to the shaded area. For clarity we only display the h<0 part of the phase diagram corresponding to a majority of heavy (\downarrow) fermions. The h>0 side is immediately obtained by the particle-hole transformation $\mu \rightarrow -\mu + U$, $h \rightarrow -h$.

Fig. 4. It is also instructive to consider the locus of $n_{\uparrow} = n_{\downarrow}/2$ on the phase diagram. At low density $(n_{\downarrow} < n_{\downarrow}^{\rm cr})$, the trimer gap is nonzero and the commensurate densities occupy a finite area of the (h, μ) plane. At higher density $(n_{\downarrow} > n_{\downarrow}^{\rm cr})$, the energy gap closes and the locus shrinks to a single line, as illustrated in the inset of Fig. 4. As the mass asymmetry increases, the trimer phase grows in size. Similar behavior is found for the gapped phases associated to all other bound states (not shown in Fig. 4). We emphasize that in all the simulations reported above we observed a uniform ground state, apart from the usual Friedel oscillations due to the open boundary conditions. Collapsed phases occur for larger values of the ratio $|U|/t_{\downarrow}$ [14].

Relevance for experiments.—Let us finally discuss how our predictions can be tested in experiments with trapped Fermi gases. The presence of shallow harmonic traps $V_{\sigma}^{\text{ho}}(z) = m\omega_{z\sigma}^2 z^2/2$ can be taken into account via local density approximation, starting from the homogeneous solution. Here m is the atom mass and $\omega_{z\sigma}$ the trapping frequencies. In order to form trimers, we require T, $\hbar\omega_{z\sigma} \lesssim E_{\rm tr}^b$, T being the temperature of the gas. For instance, consider a sample of ⁶Li atoms in a lattice with periodicity d = 250 nm and tunneling rates $t_1 = 345$ nK and $t_{\downarrow} = 0.2t_{\uparrow}$. Assuming $U = -4t_{\uparrow}$, from Fig. 1 we obtain $E_{\rm tr}^b = 0.3t_{\uparrow} = 104$ nK, well within experimental reach. The binding energy of trimers (Fig. 1) can be directly measured by rf spectroscopy [27,28]. The effective mass (inset in Fig. 1) can be obtained by measuring the frequency of the dipole oscillations of the cloud [1]. For small displacements around the equilibrium position, the kinetic energy of trimers is quadratic, $P^2/2M_{\rm tr}^*$, and the latter is simply given by $\omega_{\rm dip} = \sqrt{(\omega_{\uparrow}^2 + 2\omega_{\downarrow}^2)m/M_{\rm tr}^*}$. To enter the trimer phase at finite density, the above condition becomes more stringent, namely T, $\hbar\omega_{z\sigma} \lesssim \Delta_{tr}$. Moreover both components must be degenerate, implying $T \lesssim E_{F\uparrow}$, $E_{F\downarrow}$ where $E_{F\sigma}$ are the Fermi energies in the absence of interaction. This sets a lower bound on the values of the densities at the center of the trap. For the above choice of parameters, the best tradeoff occurs around $n_1(0) =$ $2n_{\uparrow}(0) \sim 0.3/d$ yielding T, $\hbar\omega_{z\sigma} \lesssim 60$ nK. The two spin populations should be tuned close to the commensurate point $N_{\uparrow} = N_{\downarrow}/2$, otherwise phase separation in shells will occur [6,7]. Finally, the suppression of the superconducting correlations (Fig. 3), signaling the emergence of the trimer phase, can in principle be detected using interferometric techniques, as discussed in Ref. [29].

Concluding, we have shown that 1D attractive fermions with unequal masses form trimers and other more exotic bound states. Differently from pairs, these states can only open a gap at low density or, equivalently, strong interactions. In the gapped phase FFLO superconducting correlations are exponentially suppressed. The properties of trimers in vacuum and at finite densities are experimentally accessible with ultracold atoms. The DMRG simulations were performed using the ALPS libraries [30].

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