We study the phase diagram of a one-dimensional, two-component (i.e., pseudo-“spin”-12) ultracold atomic Fermi gas. The two atom species can have different hopping or mass. A very rich phase diagram for equal densities of the species is found, containing Mott insulators and superfluids. We also discuss coupling such 1D systems and the experimental signatures of the phases. In particular, we compute the spin-structure factor at small momentum, which should reveal a spin gap.
Two-Component Fermi Gas on Internal-State-Dependent Optical Lattices

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We study the phase diagram of a one-dimensional, two-component (i.e., pseudo-“spin”-1/2) ultracold atomic Fermi gas. The two atom species can have different hopping or mass. A very rich phase diagram for equal densities of the species is found, containing Mott insulators and superfluids. We also discuss coupling such 1D systems and the experimental signatures of the phases. In particular, we compute the spin-structure factor at small momentum, which should reveal a spin gap.

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Quantum engineering [1,2] of strongly correlated many-body systems has recently become possible thanks to the spectacular advances in trapping ultracold atoms in optical lattices [3–6] or in microchip traps [7]. This has led to the study of models that would otherwise be hard to realize in solids, which may shed light on basic issues in quantum many-body physics, including the understanding of, e.g., the origin of high-\(T_c\) superconductivity in doped copper oxides. In particular, correlated boson [3,4,8,9], Bose-Fermi [10], and Fermi [11–13] systems have received much experimental and theoretical attention in recent times.

In sharp contrast to electrons in solids, in cold atomic systems, different types of atoms (different hyperfine states or different atomic species) can be trapped and controlled independently, such that the hopping, strength, and sign of interactions (inter- or intraspecies) and densities can be continuously tuned. For example, Mandel et al. [5] controlled independently the periodic potential for each atom type loaded in an optical lattice. This leads to much richer physics which remains to be understood.

In this Letter, motivated by these recent developments and the availability (now or soon) of fermions in elongated traps [6,7], we study the interesting effects of having different Fermi velocities for two species of fermions in one dimension (1D). With equal densities of the two species, this system is different from a two-leg spinless ladder [14,15] or the spin-1/2 electrons in a magnetic field [15,16]. One main result of this Letter is the phase diagram as a function of velocity difference, for equal densities (Fig. 1). With repulsive interactions, a finite velocity difference breaks the SU(2) spin [17] symmetry and turns the gapless Tomonaga-Luttinger liquid (TLL) into an Ising spin-density wave with a spin gap. Segregation of spin-up and -down fermions may occur if one type of fermions has a very tiny velocity. With attractive interactions, a singlet superfluid (SS) of bound pairs of fermions of different types gives way to a charge density wave (CDW) of pairs for sufficient velocity difference. We also briefly study the effects of a small tunneling term coupling an array of 1D tubes together. In particular, if there are different densities of fermions in neighboring tubes, a triplet superfluid (TS) may become stable for repulsive interactions. Finally, we calculated the dynamical spin structure factor to reveal the spin gap.

We study the following generalized Hubbard model:

\[
H = - \sum_{\sigma,m} t_\sigma (c_{\sigma m}^\dagger c_{\sigma m+1} + H.c.) + U \sum_m n_{m\uparrow} n_{m\downarrow}. \tag{1}
\]

![FIG. 1 (color online). Schematic phase diagram for the model of Eq. (1) with equal number of spin-up and -down fermions away from half filling (i.e., \(N_{10} = N_{1\bar{0}} \neq M/2\)). \(U\) is the interaction strength and \(z = |t_\uparrow - t_\downarrow|/(t_\uparrow + t_\downarrow)\). All phases (SDW: spin-density wave, CDW: charge density wave, SS: singlet superfluid, TS: triplet superfluid) exhibit a spin gap \(\Delta_s\), except \(\Delta_s = 0\) for \(U = 0\) (FG: Fermi gas) and \(z = 0\) for \(U > 0\) (TLL: Tomonaga-Luttinger liquid). The first acronym refers to the dominant type of order, the second (in parentheses) to the subdominant one (see text for explanations). A cartoon of the dominant order in each phase is also shown. In the area between dashed lines the dominant order (either CDW or SS) depends on the lattice filling (see text). In the SG phase, spin-up and -down fermions are segregated (demixed).](https://www.physrevlett.org/10.1103/PhysRevLett.95.226402)
This Hamiltonian describes a 1D Fermi gas on a internal-state-dependent periodic potential [5]. The local interaction $U$ arises from projecting within the lowest Bloch band the short-range two-body interaction $v(x) = g_{1D} \delta(x)$, where $g_{1D}$ is related to the s-wave scattering length by Eq. (14) of Ref. [18]. Experimentally, the system is prepared as mixture of $N_{0\sigma}$ fermions [6] (i.e., the total magnetization and particle number are fixed). The index $m = 1, \ldots, M$ labels the lattices sites, $n_{\alpha\sigma} = c_{\alpha m}^{\dagger} c_{\alpha m}$, and $\sigma = \uparrow, \downarrow$ is the spin [17] index that may refer to two hyperfine states, or two different types of atoms (e.g., $^6\text{Li}$ and $^{40}\text{K}$). Even though there may be no true spin symmetry, we use the spin language to describe this binary mixture. We assume the number of fermions of each spin species is separately conserved, i.e., one spin type cannot be converted to another. Motivated by the experimental considerations above, we allow for different hopping $t_{\sigma}$ for different spins. This Hamiltonian may be realized in either a quasi-1D chip trap [7] or in a 2D optical lattice, which is made up of an array of 1D gas tubes [4,8] weakly coupled by a hopping $t_{\perp} \ll \min(t_\uparrow, t_\downarrow)$. When the energy gained by hopping between neighboring tubes ($\propto t_{\perp}$) gets smaller than the cost of adding (or removing) an extra atom to one of the finite-sized tubes (“charging energy”), the tubes decouple from one another and a set of independent 1D tubes is recovered [19]. Although we assume there is a (spin-dependent) periodic potential parallel to the tubes such that (1) applies, many of our results also apply in the absence of this potential when the two species have different masses. More discussion on engineering Hamiltonians like (1) can be found in [1].

We first study the homogeneous 1D system in the thermodynamic limit; finite-size and trap effects are discussed below.

The weak-coupling limit $|U| \ll \min(t_\uparrow, t_\downarrow)$ can be solved by taking the continuum limit of (1) [15] and linearize the dispersion around the Fermi points $\pm k_F^\sigma = \pi N_{0\sigma} / M a$. This leads to the so-called “g-ology” representation [15] with a small number of coupling constants representing low energy scattering processes. The coupling $g_{2\parallel}$ ($g_{2\perp}$) is the scattering amplitude for processes where a small momentum $q$ is exchanged between fermions of equal (opposite) spin at opposite Fermi points, for arbitrary values of $k_F^\sigma$. $g_{1\parallel}$ is the backscattering amplitude where two fermions of opposite spin exchange a momentum $q = 2k_F = 2k_F^\uparrow = 2k_F^\downarrow$, and is relevant only when $N_{0\uparrow} = N_{0\downarrow}$; $g_{1\perp}$ is the amplitude for umklapp scattering ($q = 2k_F^\uparrow + 2k_F^\downarrow = \pi / a$) and is important only at half filling: $N_{0\uparrow} + N_{0\downarrow} = M$. Thus for generic fillings, $g_{1\parallel}$ and $g_{3\parallel}$ are irrelevant, and the system is a TLL [15] with a completely gapless spectrum of two distinct branches of phonons.

We focus here on the case $N_{0\uparrow} = N_{0\downarrow} \neq M/2$. The case of a half-filled lattice $N_{0\uparrow} = N_{0\downarrow} = M/2$ is more involved and will be reported elsewhere [19]. Unlike Refs. [20,21], we obtain the phase diagram for equal number of spin-up and -down fermions as a function of the (Fermi) velocity difference and consider coupling the 1D systems together.

The physical properties can be established by analyzing the renormalization group (RG) flow of the various scattering amplitudes upon the varying of a cutoff such as the temperature $T$. To second order in the interaction parameters, the RG flow is [19]:

$$
\dot{y}_1 = -y_1^2, \quad \dot{y}_2 = -y_2^2, \quad \dot{y}_3 = -y_3^2,
$$

(2)

where $y_\sigma = g_\sigma / \pi \hbar v$ are dimensionless couplings, $v = (v_\uparrow + v_\downarrow)$, $r_\sigma = v / 2 v_\sigma$, $y_\sigma$, and $y_2 = -\sum_{\sigma} r_\sigma y_\sigma^{2\parallel} + 2 y_2^\parallel$, $\dot{y}_\sigma = d y_\sigma / d \ell$, with $\ell = ln(A/T)$. Equations (2) can be mapped to the RG equations of the Berezinskii-Kosterlitz-Thouless (BKT) transition in terms of $y_1 \perp$ and $y_2 \perp$. The behavior of the BKT equations is determined [15] by the constant of motion $C = y_1^2 \perp - y_2^2 \perp / 2 (r_\uparrow r_\downarrow + 1) = (U a / \hbar v)^2 z^2 / (2 - z^2)$, where $z = |t_\uparrow - t_\downarrow| / (t_\uparrow + t_\downarrow)$ is the key velocity difference parameter. For $z = 0$ we recover the results for the spin-symmetric Hubbard model [15]. However, for $z \neq 0$ and $\mathcal{U} \neq 0$, $C > 0$, the scattering amplitude $y_1 \perp (\ell)$ diverges as the system is cooled down to its ground state. This signals the formation of bound states, and the opening of a gap in the spin sector (the charge excitations remain gapless). For $z \ll 1$, the gap has thus the characteristic BKT form $\Delta_s \sim \Lambda \pi^{-A} / \sqrt{v} \sim \Lambda e^{-A / |t_\uparrow - t_\downarrow|}$, where $\Lambda \sim t_\uparrow = t_\downarrow$ and $A, A'$ are constants.

Note that this gap is nonperturbative in $|t_\uparrow - t_\downarrow|$. The properties of the spin-gapped phase depend on the sign of $\mathcal{U}$. Ground states of 1D systems are characterized by the dominant form of order that they exhibit, which is typically quasi-long range in character, true long-range order being only possible in 1D when a discrete symmetry is broken. For $\mathcal{U} > 0$ and $z \neq 0$, then $y_1 \perp (\ell) \rightarrow \infty$, and a bosonization study [19] shows that the dominant order (i.e., the slowest decaying correlation) is a spin-density wave (SDW) and the subdominant order (the next slowest decaying correlation) is triplet superfluidity (TS). In the attractive case ($\mathcal{U} < 0$), as $z$ is increased, the dominant (subdominant) order changes from SS (CDW) to CDW (SS). This changeover is due to the marginal coupling between the gapless charge and the gapped spin modes, leading to the TLL parameter $K_c$, going from $K_c > 1$ to $K_c < 1$ as $z$ is increased, which changes the dominant correlations from SS to CDW, as described. A summary of the phase diagram is shown in Fig. 1.

The weak-coupling regime crosses over to the strong coupling regime $|\mathcal{U}| \gg \max(t_\uparrow, t_\downarrow)$, as confirmed by a strong coupling expansion of (1). We only give here the main steps; technical details can be found in [19]. We first consider a half-filled lattice with $N_{0\uparrow} = N_{0\downarrow} = M/2$. For $\mathcal{U} \gg \max(t_\uparrow, t_\downarrow)$ fermions cannot hop around and there is a gap of order $\mathcal{U}$ to charge excitations. Degenerate perturbation theory [22] shows that in this limit the Hamiltonian in (1) maps to the Heisenberg-Ising (XXZ) spin chain
$H_{XXZ} = J \sum_m [S_m \cdot S_{m+1} + \gamma S_m S_{m+1}^z]$, where the $S_m$ denotes the spin operator at site $m$, $J = 4t_1t_2/U$, and the anisotropy $\gamma = (t_1 - t_2)^2/2t_1t_2 \approx z^2$. Thus, for unequal hopping ($z > 0$), the chain is in the Néel phase (SDW with true long-range order), and has a spin gap which for small $z$ is $\Delta_{s} \sim J e^{-\gamma /\sqrt{5}} = J e^{-\gamma /|t_1-t_2|}$ [20]. Note the same nonperturbative dependence on $t_1 - t_2$ as for the weak-coupling regime. Away from half filling, the system is described by a $t$-$J$ model with anisotropic spin interactions. The charge gap is destroyed ($K_c = \frac{1}{2}$ close to half filling [15]), but the spin gap remains and the dominant order is still SDW. Physically, the finite velocity difference breaks the SU(2) spin symmetry to the lower $Z_2 \times U(1)$. Thus, the TLL becomes an Ising antiferromagnet in the spin sector.

For $U \ll 0$, (1) is equivalent to a model of tightly bound fermion pairs (hard-core bosons annihilated by $b^\dagger_m = c^\dagger_m c_m$). Their hopping amplitude is $J = 4t_1t_2/|U|$, and they interact with strength $V = 2(t_1^2 + t_2^2)/|U|$ when sitting at nearest-neighbor sites. This model can be mapped to the XXZ chain via $b^\dagger_m \rightarrow S^+_m$ and $(b^\dagger_m b_m - \frac{1}{2}) \rightarrow S^z_m$.

At half filling, charge excitations are gapless for equal hopping and SS is the dominant order [15]. However, with unequal hopping the spectrum of the tube is fully gapped, becoming a CDW with true long-range order, a spin gap of order $|U|$ (energy to break a pair), and a charge gap $\Delta_{c} \sim J e^{-\gamma /|t_1-t_2|}$. Away from half filling, the spin gap remains $\sim |U|$ but the bosons are able to hop (i.e., the charge gap disappears). Note that very close to half filling for $z \neq 0$, the dominant order is CDW since $K_c \rightarrow \frac{1}{2}$, as can be inferred from the exact solution of the XXZ chain [15,23]. However, as the filling deviates more and more from half filling, $K_c$ rises above one and the system becomes a 1D superfluid (SS). This change in the character of the dominant order also takes place at constant filling, provided the system is sufficiently far from half filling: a SS ($K_c > 1$) can turn into a CDW ($K_c < 1$) as $|z|$ is varied at strong coupling. This agrees with the above weak-coupling analysis. Note that at very low density ($N_{0ur}/M \rightarrow 0$), and at least for not too different velocities, only a SS phase is possible: in this limit, (1) maps to a continuum (Gaudin-Yang-like) model of interacting fermions with spin-dependent mass. For $U \rightarrow -\infty$, the fermions pair up to become a 1D superfluid (SS) of tightly bound pairs with irrelevant residual interactions between the pairs.

Finally both the weak and strong coupling analysis described above break down for sufficiently large $|t_1 - t_2|$; for weak coupling, linearization of the free fermion dispersion is no longer justified, while for large $|U|$ degenerate perturbation theory becomes subtle. Unfortunately, rigorous results are available only for $t_1 = 0$ or $t_1 = 0$ ($z = 1$), which is the Falicov-Kimball model. In 1D, Lemberger [24] [see also [25]] has proved that spin-up fermions segregate from spin-down ones for $U > U_c > 0$ at equal densities. There is no segregation for $U < 0$ at equal densities. As argued in [19,25], it is quite likely that this segregated phase will survive also when $|z|$ is close to 1.

The predicted phase diagram of Fig. 1 for a single 1D tube can be directly tested experimentally in cold atoms, but it is also interesting to analyze when there is weak tunneling between the tubes in a square 2D array of tubes [4,8]. The Hamiltonian for each tube at site $\mathbf{R}$ of the 2D lattice is as in Eq. (1), with all fermion operators now carrying the $\mathbf{R}$ label. The hopping between the nearest-neighbor tubes at $\mathbf{R}$ and $\mathbf{R}^\prime$ is described by $H_1 = -t_{\perp} \sum_{(\mathbf{R},\mathbf{R}^\prime)} \sum_{m,n} c^\dagger_{mR} c_{nR^\prime}$, where $t_{\perp} \ll \min(t_1, t_2)$, but such that fermions can now overcome the “charging energy” of the finite-size tubes. In general, when the isolated tube has a gap $\Delta_s \ll t_1$, a relevant perturbation (in the RG sense) and fermions hop coherently from tube to tube. This is likely to lead to a very anisotropic 3D Fermi liquid, which in turn may become unstable to 3D CDW or SDW formation or 3D BCS superfluidity under appropriate conditions. This limit has been much studied in the past, e.g., for organic superconductors [see [26] for a review]. We shall not consider it here, and instead we study $t_1 \neq t_2$ so that the gap $\Delta_s \gg t_1$. Since the tubes (or at least a large number of them near the center of the trap due to inhomogeneity effects) can develop a sufficiently large spin gap as described above, coherent hopping between tubes is now suppressed. However, $H_1$ can generate, through virtual transition terms of $O(t_{\perp}^4)$, of two kinds [15,27]: (i) particle-hole pair hopping generates spin-spin and density-density interactions: $H_1 = \sum_{m,(\mathbf{R},\mathbf{R}^\prime)} [J_{\perp} \sum_{m} S_{mR} \cdot S_{mR^\prime} + V_{\perp} n_{mR} n_{mR^\prime}]$, and (ii) fermion pair hopping yields $H_2 = J_{\perp} \sum_{m,(\mathbf{R},\mathbf{R}^\prime)} b^\dagger_{mR} b_{mR^\prime} + b_{mR^\prime} c_{mR} c^\dagger_{mR}$, where $J_{\perp} \simeq t_{\perp}^2/\Delta_s$, and $J_{\perp}$ is a distance smaller than the spin correlation length, $\xi_s \sim \Delta_s^{-1}$. The dominant term then drives a phase transition to a 3D ordered phase [19]: for $U < 0$, if the tubes are in the SS phase, the dominant fermion pair tunneling leads to 3D long-range SS order. The low-temperature properties of this system become identical to the superfluid of bosons studied in [8]. If the tubes are in the CDW ($U > 0$ and sufficiently large $z$) or in the SDW ($U > 0$) phases, the dominant particle-hole pair hopping leads to insulating phases that are either 3D CDW or SDW. The ordering temperatures in all cases (at small $t_{\perp}$) are power laws: $T_c \sim \Delta_s (t_1/\Delta_s)^{\alpha}$, with $\alpha^{-1} = 2(2-d)$ and $d$ the scaling dimension of the dominant intertube interaction. Interestingly, the SDW or CDW ordering is anisotropic: incommensurate (relative to the optical lattice) along the tube, but commensurate perpendicular to the tubes.

Particle-hole hopping may drive a transition to a 3D insulating state with density wave order only if the density in neighboring tubes is equal or very similar: for a particle and a hole to hop coherently at low temperatures, they must be extracted from opposite Fermi points of one tube and must match the momenta in the neighboring tube by momentum conservation. If the density mismatch between
tubes is sufficiently large, particle-hole hopping is suppressed and only the hopping of fermion pairs (which carry zero net momentum) is possible, leading to a superfluid. Interestingly, for $U > 0$, TS is the subdominant order and the suppression of particle-hole pair hopping may then lead to a 3D triplet superfluid, with $T_c$ also a power law of $t_\perp/\Delta_s$.

The phase diagram shown in Fig. 1 holds, strictly speaking, in the thermodynamic limit. In current 2D optical lattices typically $\sim 10^5$ fermions (i.e., $\sim 100$ per tube) [6, 28]) can be loaded, but we expect all predicted phases to appear. Because of the finite size, the phase boundaries will not be true phase transitions, but rather sharp crossovers. The trap can lead to phase coexistence [29, 30], local quantum criticality [29], and even suppression of criticality [30], but we are concerned here with the phases themselves and not with the quantum critical points between them. Experimentally, the imbalance in the number of spin-up and -down fermions is of the order of a few percent [6, 28], and therefore assuming $N_\up = N_\down$ should be a good approximation. Larger imbalances can lead to interesting phenomena [19].

The most important signature of the single-tube phases that we predict is the spin gap, $\Delta_s$. To probe the gap, a laser can be used to drive stimulated Raman transitions between the two hyperfine states $\sigma = \uparrow, \downarrow$. By measuring the heating of the gas due to the probing laser or the absorption and emission rate of photons from the Raman laser [31], the dynamic structure factor $S_s(q, \omega)$, which is the Fourier transform of $S_s(r, r', t) = \langle S^+ (r, t) S^- (r', 0) \rangle$, could be measured. We have computed this using the form factor approach [32], and find [19] that for $T \ll \Delta_s$, it rises from zero as $\sqrt{(\hbar \omega)^2 - (2\Delta_s)^2}$ for $\hbar \omega \approx 2\Delta_s$. Note that this is very different from the one expected for a 3D superfluid due to the spin anisotropy induced by the hopping difference.

Concerning the coupled tubes, the most exotic phase is the triplet superfluid (TS). To “engineer” it, we need to make the number of fermions in neighboring tubes sufficiently different [33]. This could be achieved with a bi-periodic optical potential in the direction perpendicular to the tubes. The coherence properties of the 3D superfluid phases could be probed by exciting low frequency collective modes in the transverse direction [4] to the tubes and observing the coherent oscillations.

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[17] We use spin to refer to internal (hyperfine or species) states of the fermions. The real spin of the atoms is fixed by the experimental preparation of the mixture [6, 28].
[27] As cold atoms interact via a Dirac delta potential, there is no direct interaction between atoms in different tubes.