Spin-$\frac{1}{2}$ fermions on spin-dependent optical lattices

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We study the phase diagram of one dimensional spin-$\frac{1}{2}$ fermionic cold atoms. The two “spin” species can have different hopping or mass. The phase diagram at equal densities of the species is found to be very rich, containing Mott insulators and superfluids. We also briefly discuss coupling 1D systems together, and some experimental signatures of these phases. In particular, we compute the spin structure factor for small momentum, which should allow the spin gap to be detected.

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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, 4, 5 or in microchip traps 6. 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, 5, Bose-Fermi 10, and Fermi 11, 12, 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 intra-species) and densities can be continuously tuned. For example, Mandel et al. 3 managed to control independently the periodic potential for each atom type loaded in an optical lattice. A p-wave Feshbach resonance 14 can create a tunable asymmetry in the interactions in a multi-species Fermi gas. All this, of course, leads to a much richer physics, which remains to be understood.

In this paper, motivated by these recent developments and the availability (now or soon) of fermions in elongated traps 3, 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 the case of a two-leg spinless ladder 15, 21 or the spin-$\frac{1}{2}$ electrons in a magnetic field 16, 21. One main result of this paper 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 symmetry and turns the gapless Tomonaga-Luttinger liquid (TLL) into an Ising spin-density wave with a spin gap. Demixing 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 may give 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 describe how to detect the spin gap in these phases by measuring the dynamical spin structure factor, which we have computed. In contrast to previous studies 22, 23, we have worked out the phase diagram for equal number of spin up and down fermions as a function of the (Fermi) velocity difference and considered coupling the 1D systems together.

We study the following generalized Hubbard model:

$$H = - \sum_{\sigma, m} t_{\sigma} \left( c_{\sigma m}^\dagger c_{\sigma m+1} + \text{H.c.} \right) + U \sum_m n_{\uparrow m} n_{\downarrow m}. \quad (1)$$

This Hamiltonian describes a 1D Fermi gas with contact interactions (related to $U$) prepared with $N_{\sigma}$ fermions (i.e. we work in the canonical ensemble) and loaded in a 1D optical lattice with $m = 1, \ldots, M$ lattice sites; $n_{\sigma m} = c_{\sigma m}^\dagger c_{\sigma m}$, and $\sigma = \uparrow, \downarrow$ is the spin index that may refer to two hyperfine states, or to e.g. 6Li and 40K. Even though there may be no true spin symmetry, we will continue to use the spin (and magnetic) 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 5 or in a 2D optical lattice, which is made up of an array of 1D gas tubes 6, 8 weakly coupled by a hopping $t_\perp \ll \min\{t_\uparrow, t_\downarrow\}$. When the finite “charging energy” (due to the finite length of each tube) exceeds the renormalized hopping $E_I \propto t_\perp$, the tubes are decoupled from one another and a set of independent 1D tubes is recovered 8. Although we assume there is a (spin-dependent) periodic potential parallel to the tubes such that 14 applies, much of what is discussed below also applies in the absence of this potential when the two species have different masses. More discussion on engi-
neering Hamiltonians like [11] can be found in [11].

We first study the homogeneous 1D system in the thermodynamic limit. Finite-size and trap effects will be discussed below in connection with possible experiments.

The weak coupling limit \(|U| \ll \min\{t_\uparrow, t_\downarrow\}\) can be solved by taking the continuum limit of [11] in the standard way [21] and linearize the dispersion around the Fermi points \(\pm k_F^\uparrow = \pi N_\sigma / Ma\) (\(M\) is the number of lattice sites in the tube). This leads to the so-called “gology” representation [21] with a finite number of coupling constants representing low energy scattering processes. The coupling \(g_{2\uparrow}^\downarrow (g_{2\downarrow})\) 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 \(k_F^\uparrow\). On the other hand, \(g_{1\uparrow}\) is the back-scattering amplitude where two fermions of opposite spin exchange a momentum \(q \approx 2k_F^\uparrow = 2k_F^\downarrow = 2k_F^2\), and is relevant only when \(N_{\uparrow\uparrow} = N_{\downarrow\downarrow}\); \(g_{3\uparrow}\) is the amplitude for umklapp scattering \((q \approx 2k_F^\uparrow + 2k_F^\downarrow = \pi/a)\) and is important only at half-filling: \(N_{\uparrow\uparrow} + N_{\downarrow\downarrow} = M\). Thus for generic fillings, \(g_{1\uparrow}\) and \(g_{3\uparrow}\) are irrelevant, and the system is a TLL [21], which has a completely gapless spectrum of two distinct branches of phonons.

We focus here on the case \(N_{\uparrow\uparrow} = N_{\downarrow\downarrow} \neq M/2\). The case of a half filled lattice \(N_{\uparrow\uparrow} = N_{\downarrow\downarrow} = M/2\) is more involved and will be reported elsewhere [17].

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 [17]:

\[
\begin{align*}
\dot{y}_{2\uparrow} &= r - \sigma y_{2\uparrow}^2, \\
\dot{y}_{2\downarrow} &= -y_{2\downarrow}^2, \\
\dot{y}_{1\uparrow} &= (r_{\uparrow} y_{2\uparrow} + r_{\downarrow} y_{2\downarrow} - 2y_{2\uparrow}) y_{1\uparrow},
\end{align*}
\]

where \(y_\sigma = g_\sigma / \pi \hbar v\) are dimensionless couplings, \(v = (v_\uparrow + v_\downarrow)/2\) the mean velocity and \(r_\sigma = v/2v_\sigma, \ y_\sigma = dy_\sigma / d\ell\), with \(\ell = \ln(\Lambda/T)\). Eqs. [23] can be mapped to the RG equations of the Berezinskii-Kosterlitz-Thouless (BKT) transition in terms of \(y_{2\uparrow} = -\sum_\sigma r_\sigma y_\sigma^2 + 2y_{2\uparrow}\) and \(y_{1\uparrow}\). The behavior of the BKT equations is entirely determined [21] by the constant of motion \(C = y_{1\uparrow}^2 - y_{2\uparrow}^2 / (2r_{\downarrow} + 1) = (Ua/\hbar v)^2 z^2 / (2 - z^2),\) where \(z = |t_{\uparrow\uparrow} - t_{\downarrow\downarrow}|/(t_{\uparrow\uparrow} + t_{\downarrow\downarrow})\) is the key velocity difference parameter. For \(z = 0\) we recover the well-known results for the spin-symmetric Hubbard model [21]. However, for \(z \neq 0\) and \(U \neq 0, C > 0\), the scattering amplitude \(y_{1\uparrow}(\ell)\) 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 \(\Delta \sim \Lambda \exp(-1/\sqrt{\pi \Lambda}) \approx \Lambda \exp(-A' / |t_{\uparrow\uparrow} - t_{\downarrow\downarrow}|),\) where \(\Lambda\) is of the order of the \(t_{\uparrow\uparrow} \approx t_{\downarrow\downarrow}\) and \(A, A'\) are constants. Note that this gap is non-perturbative in \(|t_{\uparrow\uparrow} - t_{\downarrow\downarrow}|\).

The properties of the spin-gapped phase depend on the sign of \(U\). 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 \(U > 0\) and \(z \neq 0\), then \(y_{1\uparrow}(\ell) \rightarrow \infty\), and a bosonization study [17] shows that the dominant order is a spin-density wave (SDW) and the subdominant order is triplet superfluidity (TS). In the attractive case \((U < 0)\), as \(z\) is increased, the dominant order changes from a singlet superfluid phase (SS) to a charge density wave (CDW), with CDW and SS being the subdominant order in the former and latter case, respectively. We wish to point out that our analysis takes fully into account the marginal (in the RG sense) coupling between the gapless charge and the gapped spin modes arising at \(z \neq 0\), which leads to an often substantial decrease in the value of the Luttinger-liquid parameter \(K_\sigma \) (proportional to the charge compressibility). In particular, for \(U < 0\) we find that \(K_\sigma \) goes from \(K_\sigma > 1\) to \(K_\sigma < 1\) as \(z\) is increased, which changes the character of the dominant correlations from SS to CDW, as described above.

A summary of the phase diagram is shown in Fig. 1.
The weak-coupling regime smoothly crosses over to the strong coupling regime \(|U| \gg \max\{t_\uparrow, t_\downarrow\}\), as confirmed by a strong coupling expansion of \(|\Omega|\). We only give here the main steps, technical details can be found in \([17]\). It is simplest to first consider a half-filled lattice with \(N_{\uparrow 0} = N_{\downarrow 0} = M/2\). For the strongly repulsive case \(U \gg \max\{t_\uparrow, t_\downarrow\}\) fermions cannot hop around and there is a gap of order \(U\) to charge excitations. Degenerate perturbation theory \([13]\) then shows that in this limit the Hamiltonian in \([\Omega]\) maps to the Heisenberg-Ising (XXZ) spin chain \(H_{\text{XXZ}} = J \sum_m [S_m \cdot S_{m+1} + \gamma z_m \cdot z_{m+1}]\), where the \(S_m\) denotes the spin operator at site \(m\), \(J = 4t_\uparrow t_\downarrow / U\), and the anisotropy \(\gamma = (t_\uparrow - t_\downarrow)^2 / 2t_\uparrow t_\downarrow \propto z^2\). Thus, for unequal hopping \((z > 0)\), the chain is in the Neel phase (SDW with strong long-range order), and has a spin gap which for small \(z\) is \(\Delta_s \sim J e^{-A^s / \sqrt{\gamma}} = J e^{-A^s / |t_\uparrow - t_\downarrow|}\) \([22]\). Note the same non-perturbative dependence on \(t_\uparrow - t_\downarrow\) as for the weak coupling regime. Away from half-filling, the system is described by a \(t-J\)-like model with anisotropic spin interactions. The charge gap is destroyed \((K_c = \frac{1}{2}\) close to half-filling \([21]\), 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 anti-ferromagnet in the spin sector.

For \(U \ll 0\), degenerate perturbation theory shows that \([\Omega]\) is equivalent to a model of tightly bound fermion pairs (hard-core bosons) annihilated by \(b_m = c_m^\dagger c_m\). Their hopping amplitude is \(J = 4t_\uparrow t_\downarrow / |U|\), and they interact with strength \(V = 2(t_\uparrow^2 + t_\downarrow^2) / |U|\) when sitting at nearest-neighbor sites. This model can be mapped to the above XXZ chain via \(b_m \rightarrow S_m^-\) and \((b_m^\dagger b_m - \frac{1}{2}) \rightarrow S_m^z\). At half-filling, charge excitations are gapless for equal hopping and SS is the dominant order \([21]\). 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 \(\Delta_c \sim J e^{-A^c / |t_\uparrow - t_\downarrow|}\). Away from half-filling, the spin gap remains \(\sim |U|\) but the bosons are able to hop (i.e. the charge gap disappears). It is worth pointing out 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 \([21, 26]\). 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 \((N_{\uparrow 0}/M \rightarrow 0)\), and at least for not too different densities, only a SS phase is possible: in this limit, \([\Omega]\) 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 \(|t_\uparrow - t_\downarrow|\). For weak coupling, linearization of the free fermion dispersion is no longer justified when \(t_\uparrow \gg t_\downarrow\) (or viceversa), that is, for \(z \rightarrow 1\). In the large \(|U|\) limit degenerate perturbation theory becomes quite subtle. Unfortunately, rigorous results are available only for \(t_\uparrow = 0\) or \(t_\downarrow = 0\) \((z = 1)\), which is the limit of the Falicov-Kimball model. In 1D, Lemberger \([10]\) (see also \([20]\)) has proved that spin up fermions segregates 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 \([14, 20]\), it is quite likely that this segregated phase will survive also when \(|z|\) is not one but close to one.

The predicted phase diagram of Fig. \([1]\) for a single 1D tube can be directly tested experimentally in cold atoms. However, it is also interesting to analyze the case when the tubes are weakly coupled by tunneling between the tubes. We thus briefly describe the phase diagram for an array of coupled 1D tubes in a 2D optical lattice geometry \([4, 8]\). The Hamiltonian for each tube at site \(R\) of the 2D lattice is as in Eq. \([\Omega]\), with all fermion operators now carrying the \(R\) label. The hopping between the nearest neighbor tubes at \(R\) and \(R'\) is described by \(H_\perp = -t_\perp \sum_{\langle R,R' \rangle} \sum_{\sigma,m} c_m^\dagger \sigma c_m R c_{\sigma R'}\), where \(t_\perp \ll \min\{t_\uparrow, t_\downarrow\}\), but such that fermions can now overcome the ‘charging energy’ of the finite-size tubes. In general, when the isolated tube has a gap \(\Delta_s \ll t_\perp\), \(H_\perp\) is a relevant perturbation (in the RG sense) that leads to coherent hopping of fermions from tube to tube. Thus the ground state will most likely be a very anisotropic 3D Fermi liquid, which in turn may become unstable to 3D CDW/SDW formation or 3D BCS superfluidity under appropriate conditions. This limit has been much studied in the past \(e.g.\) in connection with organic superconductors (see \([24]\) for a review). We shall not consider it here, and instead we study \(t_\perp \neq t_\parallel\) so that the gap \(\Delta_c > t_\perp\).

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, the term \(H_\perp\) can generate, through virtual transitions which are second order in \(t_\perp\), intertube interactions of two kinds \([21]\): i) particle-hole pair hopping generates spin-spin and density-density interactions: \(H_1 = \sum_{\langle R,R' \rangle} \{J_{\perp} S_{R \parallel} \cdot S_{R' \parallel} + V_{\perp} n_{R \parallel} n_{R' \parallel}\}\), ii) fermion pair hopping yields \(H_2 = J_{c \perp} \sum_{\langle R,R' \rangle} b_{R \parallel}^\dagger b_{R' \parallel} + j_{\perp}^\dagger \sum_{\langle R,R' \rangle} b_{R \parallel}^\dagger b_{R' \parallel} + j\), where \(V_{\perp}, J_{c \perp} \sim t_\perp^2 / \Delta_s\), \(b_{R \parallel} = c_{R \parallel}^\dagger c_{R \parallel}\) and \(j_a \simeq j_a^\perp \ll \xi_s \simeq \Delta_s^{-1}\). The dominant term then drives a phase transition to a 3D ordered phase \([17]\): for the \(U < 0\) case, if the tubes are in the SS phase, then the dominant process is fermion pair tunneling, and the tubes develop 3D long-range
superfluid order. The low-temperature properties of this system become identical to the superfluid of bosons studied in $\mathcal{R}$. However, if the tubes are in the CDW ($U < 0$ and sufficiently large $z$) or in the SDW ($U > 0$) phases, the dominant interactions arise from hopping of particle-hole pairs and lead to insulating phases that are either 3D CDW or SDW. The ordering temperatures in all cases (at small $t_{\perp}$) are power-laws: $T_c \propto \Delta_s(t_{\perp}/\Delta_s)^{\alpha}$, with $\alpha^{-1} = 2(2 - d)$ and $d$ the scaling dimension of the dominant inter-tube interaction. Interestingly, the SDW or CDW ordering is anisotropic: incommensurate (relative to the optical lattice) along the tube, but commensurate perpendicular to the tube direction.

Particle-hole hopping may drive a transition to a 3D insulating state with density wave order only if the density in neighboring tubes are 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 mismatch in the density between tubes is sufficiently large, particle-hole hopping is suppressed and only the hopping of fermion pairs (which carry zero net momentum) is possible. The system will then order as a superfluid. Interestingly, for $U > 0$, TS is the subdominant order in the spin gapped phase of the tubes. Suppression of particle-hole pair hopping may then lead to a 3D triplet superfluid. We note that $T_c$ for these cases is also a power law of $t_{\perp}/\Delta_s$.

The phase diagram shown in Fig. 1 holds, strictly speaking, in the thermodynamic limit. In real 2D optical lattices only a finite number of fermions ($\sim 10^5$) can be loaded, but we expect all predicted phases to appear. Due to the finite size, the phase boundaries will not correspond to true phase transitions, but rather to sharp crossovers. The trap can lead to phase coexistence and even to suppression of quantum criticality [26], but we are concerned here with the phases themselves and not with the quantum critical points between them.

The most important signature of the single tube phases that we predict is the existence of a spin gap, $\Delta_s$. By measuring the absorption of a laser that causes Raman transitions between the two hyperfine states $\sigma = \uparrow, \downarrow$, it should be possible to measure $\Delta_s$ the small momentum limit of the dynamic structure factor $S_{\sigma}(\mathbf{q}, \omega)$, which is the Fourier transform of $S_{\sigma}(\mathbf{r}, \mathbf{r'}, t) = \langle S^+_{\sigma}(\mathbf{r}, t)S^-_{\sigma}(\mathbf{r'}, 0) \rangle$. Using the so-called form factor approach [28], we find [17] that at $T \ll \Delta_s$, the structure factor rises from zero as $\sqrt{|\hbar \omega|^2 - (2\Delta_s)^2}$ for $\hbar \omega \geq 2\Delta_s$.

Concerning the coupled tubes, the most exotic phase is of course the triplet superfluid (TS). To ‘engineer’ it, we need to suppress particle-hole hopping by making the number of fermions in neighboring tubes sufficiently different. This could be achieved by imposing a rapid spatial variation of the trap potential, or better, by means of a biperiodic 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 to the tubes. Coherent oscillations should exist only in the superfluid phases and not in the insulators.

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