Confinement vs Deconfinement of Cooper Pairs in One-Dimensional Spin-3/2
Fermionic Cold Atoms

S. Capponi, G. Roux, P. Azaria, E. Boulat, and P. Lecheminant

1Laboratoire de Physique Théorique, Université Paul Sabatier, CNRS, 118 Route de Narbonne, 31400 Toulouse, France.
2Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, CNRS, 2 Avenue Adolphe Chauvin, 95302 Cergy-Pontoise, France.
3Laboratoire de Physique Théorique, Université Pierre et Marie Curie, CNRS, 4 Place Jussieu, 75005 Paris, France.
4Laboratoire MPQ, Université Paris 7, CNRS, 2 Place Jussieu, 75005 Paris, France.

(Dated: July 2, 2018)

The phase diagram of spin-3/2 fermionic cold atoms trapped in a one-dimensional optical lattice is investigated at quarter filling (one atom per site) by means of large-scale numerical simulations. In full agreement with a recent low-energy approach, we find two phases with confined and deconfined Cooper pairs separated by an Ising quantum phase transition. The leading instability in the confined phase is an atomic-density wave with subdominant quartet superfluid instability made of four fermions. Finally, we reveal the existence of a bond-ordered Mott insulating phase in some part of the repulsive regime.

PACS numbers: 67.90.+z, 05.30.Fk, 03.75.Ss, 71.10.Fd

Loading cold atomic gases into optical lattice allows for the realization of bosonic and fermionic lattice models and the experimental study of exotic quantum phases. Ultracold atomic systems also offer an opportunity to investigate the effect of spin degeneracy since the atomic total angular momentum \( F \) can be larger than 1/2 resulting in \( 2F+1 \) hyperfine states. This high-spin physics is expected to stabilize novel exotic phases. In this respect, various superfluid condensates, Mott insulating phases, and interesting vortex structures have been found in spinor bosonic atoms with \( F \geq 1 \). These theoretical predictions might be checked in the context of Bose-Einstein condensates of sodium, rubidium and in spin-3-atom of \(^{52}\text{Ce} \). The spin-degeneracy in fermionic atoms is also expected to give rise to some interesting superfluid and Mott phases. In particular, a molecular superfluid phase might be stabilized where more than two fermions form a bound state. Though such non-trivial superfluid behavior has been previously found in different contexts, it has been advocated recently that the formation of bound-state of Cooper pairs is likely to occur in general half-integer \( F > 1/2 \) ultracold atomic fermionic systems. In the spin \( F = 3/2 \) case, it has been predicted on the basis of a low-energy study in one dimension that a quartetting superfluid phase, i.e. a bound-state of two Cooper pairs, might be stabilized by strong enough attractive interactions. The simplest lattice Hamiltonian to describe spin-3/2 atoms with s-wave scattering interactions in 1D optical lattice takes the form of a Hubbard-like model:

\[
\mathcal{H} = -t \sum_{i,\alpha} [c_{\alpha,i} \dagger c_{\alpha,i+1} + \text{H.c.}] + U_0 \sum_i P_{00,i}^\dagger P_{00,i} + U_2 \sum_{i,m} P_{2m,i}^\dagger P_{2m,i},
\]

where \( c_{\alpha,i} \dagger \) is the fermion creation operator corresponding to the four hyperfine states \( \alpha = \pm 1/2, \pm 3/2 \). The singlet and quintet pairing operators in Eq. (1) are defined through the Clebsch-Gordan coefficient for two indistinguishable particles: \( P_{JM,i}^\dagger = \sum_{\alpha\beta} \langle J,M,F;\alpha\beta | F,F;\alpha\beta \rangle c_{\alpha,i}^\dagger c_{\beta,i}^\dagger \).

As it appears, it is more enlightening to express model (1) in terms of the density \( n_i = \sum_{\alpha} c_{\alpha,i}^\dagger c_{\alpha,i} \) and the singlet pairing operator \( P_{00,i}^\dagger = P_i^\dagger = \frac{1}{\sqrt{2}}[c_{1/2,i}^\dagger c_{-1/2,i} - c_{-1/2,i}^\dagger c_{1/2,i}] \):

\[
\mathcal{H} = -t \sum_{i,\alpha} [c_{\alpha,i}^\dagger c_{\alpha,i+1} + \text{H.c.}] + \frac{U}{2} \sum_i n_i^2 + V \sum_i P_i^\dagger P_i, \tag{2}
\]

with \( U = 2U_2 \) and \( V = U_0 - U_2 \). Model (2) generically displays an exact SO(5) extended spin symmetry and an SU(4) symmetry in the particular case \( U_0 = U_2 \), i.e. \( V = 0 \). In sharp contrast with the spin \( F = 1/2 \) case where both interacting terms in Eq. (2) are proportional, these terms are independent for \( F = 3/2 \) and strongly compete. While the V-term favors the pairing of two fermions for negative V, an attractive U-interaction might favor the formation of a quartet \( Q_i = c_{-1/2,i}^\dagger c_{-1/2,i} + c_{1/2,i}^\dagger c_{1/2,i} \). In fact, it has been recognized in Ref. that the above competition reveals itself through a non-trivial discrete symmetry of the problem. Indeed, model (2) possesses, on top of the SO(5) symmetry, a \( \mathbb{Z}_2 \) discrete symmetry \( U_c : c_{\alpha,i} \rightarrow e^{i\pi/2}c_{\alpha,i} \) which plays a crucial role in the low-energy physics since, as \( P_i \) is odd under \( U \), the formation of a quasi-long range BCS phase requires \( U \) to be spontaneously broken. When \( U \) is unbroken the BCS instability is strongly suppressed and the leading superfluid instability is made of four fermions i.e. a quartet which is even under \( U \). Such a two-phase structure has been recently predicted away from half-filling in the weak coupling limit by means of a low-energy approach.
In this letter, we investigate numerically the phase diagram of model (2) for $V \leq 0$ at quarter filling (one atom per site) by means of quantum Monte-Carlo (QMC) and Density-Matrix Renormalization Group (DMRG) simulations. Physical properties are investigated by computing the one-particle, density, pairing as well as quartetting correlation functions, respectively: $G(x) = \langle c_{\alpha,i}^\dagger c_{\alpha,i+x} \rangle$, $N(x) = \langle n_i n_{i+x} \rangle$, $P(x) = \langle P_i P_{i+x}^\dagger \rangle$ and $Q(x) = \langle Q_i Q_{i+x}^\dagger \rangle$. For the QMC simulations, we used the projector auxiliary field QMC algorithm (see Ref. 12 for the details of the algorithm) in the regime $V \leq 0$ and $U \leq -3V/4$ where the fermionic algorithm has no sign problem. We have studied periodic chains with linear size up to $L = 180$ with a typical projection parameter $\Theta t = 10$ and a Trotter time slice $\Delta t = 0.05$. Most of DMRG calculations were performed on open chains with $L = 60$ sites and keeping $M = 1400$ states. The resulting phase diagram at quarter filling is presented in Fig. 1 and we now turn to the discussion of the physical properties of the different phases.

**Confined Phase** – The phase with $U < 0$ and small $|V|$ is characterized by the existence of a spin gap and an unbroken $\mathbb{Z}_2$ discrete symmetry $\mathcal{U}$ which marks the onset of an Atomic Density Wave (ADW) and quartet superfluid quasi-long-range orderings. Indeed, for the typical value of $U = -1.5t$ and $V = 0$, we observe in Fig. 2(b) that both the pairing correlations and the one-particle Green function decay exponentially with distance. In contrast, the quartet correlations are algebraic as it can be seen in Fig. 2(a). We have checked by a direct evaluation that the four-particle gap vanishes. We can thus deduce that the short-range character of $P(x) \sim P(x)^\dagger$. (b) Short-range behavior of the one-particle Green function.

**ADW**

![Figure 1](image1.jpg)

**DMRG**

![Figure 2](image2.jpg)

![Figure 3](image3.jpg)

![Figure 4](image4.jpg)
where the factor 4 comes from the four spin states. This procedure has been shown to be very accurate for the spin-1/2 Hubbard model. For DMRG calculations, $K_d$ can be independently obtained from the power-law behavior of the quartet correlations $Q(x)$. Both QMC and DMRG results are shown for example on the SU(4) invariant line ($V = 0$) in Fig. 5(a). We find that QMC works better than DMRG in the weak coupling limit and is in excellent agreement with the perturbative estimate: $K_d^2 = 1 + [V + 3U]/(2\pi x)^2$. For larger $|U|$, DMRG is more accurate and we found that $K_d$ saturates at the value $K_d \simeq 1.6$. Note that the perturbative estimate fails beyond $|U| \geq t$ so that numerical approaches become necessary to estimate $K_d$. For $V \neq 0$, $K_d$ also saturates at strong couplings to values smaller than 2. We therefore conclude that, though the quartet correlations are quasi-long ranged, the dominant instability in the confined phase is a $2k_F$-ADW.

**Deconfinement Phase** – By allowing $V$ to be sufficiently negative, one can enter a second phase where the one-particle gap is still finite (see Fig. 4(b)) for $U = 0$, $V = -3t$ but the two-particle gap vanishes. In this phase, pairing correlations become algebraic with $P(x) \sim x^{-1/2K_d}$ as shown on Fig. 4(a) and $Q(x)$ remains critical with $Q(x) \sim P(x)^4$ which is the prediction of the low-energy approach. In contrast to the ADW phase, there is no diverging signal at $2k_F = \pi/2$ in $N(q)$ (see Fig. 5(a)). We thus conclude that there is still a spin-gap and the $Z_2$ symmetry $U$ is now spontaneously broken which leads to the formation of a quasi-long-range BCS phase. In addition, there is also an ADW instability at $4k_F = \pi$ (see Fig. 5(a)) where $N(q)$ has a maximum at $q = \pi$ which has a power-law decay $N(x) \sim \cos(\pi x)x^{-2K_d}$. We thus need to compute numerically $K_d$ to fully characterize the dominant instability of this phase. As in the previous phase, the Luttinger parameter $K_d$ can be extracted either from Eq. (3) (QMC) or from pairing correlations (DMRG). As shown on Fig. 5(b), both results are compatible and agree with the perturbative estimate when $|V| < t$. We find that $K_d > 1/2$ so that the dominant instability in this phase is the BCS singlet pairing.

**Quantum phase transition** – The striking feature of the phase diagram for attractive $U$, $V$ interactions is the change of status of the $Z_2$ symmetry $U$ which is spontaneously broken (resp. unbroken) in the deconfined (resp. confined) phase. We thus expect a quantum phase transition in the Ising universality class between these two phases. In fact it has been shown in Ref. 6 that the order parameter $\sigma(x)$ associated with the $U$ symmetry, though being non-local in terms of the lattice fermions, can be extracted from the long-distance behavior of the ratio $R(x) = P(x)^4/Q(x)$. In the confined phase where $U$ is unbroken, $\langle \sigma(x) \rangle = 0$ and $R(x) \sim \langle \sigma(x)\sigma(0) \rangle^4$ decays exponentially with distance. In the deconfined phase, $\langle \sigma(x) \rangle = \sigma \neq 0$ and $R(x) \sim \sigma^8$. Finally, it has been found in Ref. 6 that at the transition the ratio displays an universal power-law behavior: $R(x) \sim 1/x$. We have computed numerically this ratio by DMRG for various parameters to determine the transition line in Fig. 6.

The results of Fig. 5(a) clearly show an excellent agreement with the predictions of the low-energy approach.
In particular, we observe that $R(x) \sim 1/x$ near the critical point. In the deconfined phase, $R(x)$ saturates at large distance as it should and is almost independent of $x$ ($R(x) \sim \sigma(U)^{\frac{1}{6}}$) when one enters the critical regime (for $U_c \leq U \leq U^*$ in Fig. 4(b)). The plot in Fig. 4(c) demonstrates that $\sigma(U) \sim (U - U_c)^{1/4}$ in full agreement with Ising criticality. In this respect, the situation is in sharp contrast with the $F = 1/2$ well-known case where the $2k_F$-ADW and BCS instabilities coexist for attractive interaction.

**Mott phase** – At quarter-filling, a Mott transition might take place if $K_d < 1/2$ with the formation of a density gap\(^5\). For the repulsive SU(4) Hubbard chain ($V = 0$), the QMC study of Ref. 16 found a transition from a gapless spin-density wave (SDW) to a generalized Mott SDW with three gapless spin modes (see Fig. 1). For $V < 0$, we expect an entirely different Mott phase due to the presence of a spin gap and the breaking of the $Z_2$ symmetry $U$. In the Mott region in Fig. 1 (full circles), the BCS singlet pairing becomes short-ranged as shown in Fig. 4(a) and we find that, as the density gap opens, the local density almost does not fluctuate and $N(x) \sim 1$. In contrast, the local kinetic bond, $t(x) = \langle \sum_{\alpha} c_{\alpha,x+1}^\dagger c_{\alpha,x} + \text{H.c.} \rangle$, orders with a $4k_F = \pi$ modulation reminiscent of a *doubly degenerate* ground state as it can be seen in Fig. 7(b-d) for $V = -2t$. We therefore conclude on the emergence of a bond-ordering Mott phase with periodicity two (Mott BOW in Fig. 1).

**Concluding remarks** – We conclude this letter in emphasizing that the existence of a quartet superfluid phase where quartet correlations dominate over the $2k_F$-ADW instability relies on the non-universal Luttinger parameter $K_d$. Though $K_d < 2$ at quarter filling, we expect that at sufficiently low densities, $K_d$ may become larger than 2, which marks the onset of the quartetting phase. The formation of this exotic phase will be discussed in a forthcoming paper.

**Acknowledgments**

We would like to thank K. Totsuka, C. J. Wu, and S.-C. Zhang for useful discussions. S. C. and G. R. thank IDRIS (Orsay, France) and CALMIP (Toulouse, France) for use of supercomputer facilities, and Agence Nationale de la Recherche (France) for support.

---

* Electronic address: capponi@irsamc.ups-tlse.fr
1. M. Lewenstein et al., arXiv: cond-mat/0606771
2. T.-L. Ho, Phys. Rev. Lett. 81, 742 (1998).
3. T. Ohmi and K. Machida, J. Phys. Soc. Jpn. 67, 1822 (1998); F. Zhou and G. W. Semenoff, Phys. Rev. Lett. 97, 180411 (2006); R. Barnett, A. Turner, and E. Demler *ibid.*, 180412 (2006); R. B. Diener and T.-L. Ho, *ibid*. 96, 190405 (2006).
4. J. Stenger *et al*., Nature (London) 396, 345 (1998); M. S. Chang *et al*., Nature Phys. 1, 111 (2005); A. Griesmaier et al., Phys. Rev. Lett. 94, 160401 (2005).
5. P. Schlottmann, J. Phys. Condens. Matter 6, 1359 (1994); G. Röpke, A. Schnell, P. Schuck, and P. Nozières, Phys. Rev. Lett. 80, 3177 (1998); B. Douçot and J. Vidal, *ibid*. 88, 227005 (2002).
6. P. Lecheminant, E. Boulat, and P. Azaria, Phys. Rev. Lett. 95, 240402 (2005).
7. C. J. Wu, Phys. Rev. Lett. 95, 266404 (2005).
8. H. Kamei and K. Miyake, J. Phys. Soc. Jpn. 74, 1911 (2005); A. S. Stepanenko and J. M. F. Gunn, arXiv: cond-mat/9901317
9. C. J. Wu, J. P. Hu, and S.-C. Zhang, Phys. Rev. Lett. 91, 186402 (2003); C. J. Wu, Mod. Phys. Lett. B 20, 1707 (2006).
10. D. Controzzi and A. M. Tsvelik, Phys. Rev. Lett. 96, 097205 (2006).
11. S. R. White, Phys. Rev. Lett. 69, 2863 (1992); Phys. Rev. B 48, 10345 (1993). U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005).
12. F. F. Assaad, M. Imada, and D. J. Scalapino, Phys. Rev. B 56, 15001 (1997).
13. Note that the drop of correlations for the largest distances is due to a finite $M$ effect and the use of open chains. DMRG is also known to slightly underestimate correlations (and consequently $K_d$ in this study).
14. S. Ejima, F. Gebhard, and S. Nishimoto, Europhys. Lett. 70, 492 (2005).
15. A. O. Gogolin, A. A. Nersesyan, and A. M. Tsvelik, *Bosonization and Strongly Correlated Systems* (Cambridge University Press, Cambridge, England, 1998); T. Giamarchi, *Quantum Physics in One Dimension* (Clarendon press, Oxford, UK, 2004).
R. Assaraf, P. Azaria, M. Caffarel, and P. Lecheminant, Phys. Rev. B 60, 2299 (1999).