Pairing and pair superfluid density in one-dimensional Hubbard models

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We use unbiased computational methods to elucidate the onset and properties of pair superfluidity in two-species fermionic and bosonic systems with onsite interspecies attraction loaded in one-dimensional optical lattice. We compare results from quantum Monte Carlo (QMC) and density matrix renormalization group (DMRG), emphasizing the one-to-one correspondence between the Drude weight tensor, calculated with DMRG, and the various winding numbers extracted from the QMC. Our results show that, for any nonvanishing attractive interaction, pairs form and are the sole contributors to superfluidity, there are no individual contributions due to the separate species. For weak attraction, the pair size diverges exponentially, i.e. Bardeen-Cooper-Schrieffer (BCS) pairing requiring huge systems to bring out the pair-only nature of the superfluid. This crucial property is largely overlooked in many studies, thereby misinterpreting the origin and nature of the superfluid. We compare and contrast this with the repulsive case and show that the behavior is very different, contradicting previous claims about drag superfluidity and the symmetry of properties for attractive and repulsive interactions. Finally, our results show that the situation is similar for soft core bosons: superfluidity is due only to pairs, even for the smallest attractive interaction strength compatible with the largest system sizes that we could attain.

\textbf{Introduction:} Multi-component quantum systems have long attracted interest be they bosonic, fermionic or mixtures thereof. Andreev and Bashkin\textsuperscript{1} considered a two component mixture of $^4$He and superfluid (SF) $^3$He and showed that, in addition to the superflows of the individual components, there is a “drag” superfluid (DSF) density caused by the repulsive interaction between the $^4$He atoms and the Cooper pairs formed by the $^3$He. Interest in such systems increased with the experimental realization of trapped ultra-cold bosonic and fermionic atoms and mixtures of the two. The system parameters in such experiments, such as relative densities and interaction strength, are highly tunable and can be studied in the bulk or loaded in optical lattices. In this context, DSF was demonstrated with a microscopic model of a weakly interacting dilute gas in the bulk\textsuperscript{2,4} and on optical lattices\textsuperscript{2,4}. In the bulk or at low densities on a lattice, the DSF flow is along the SF flow of the separate components. However, when the coupling is strongly repulsive and the lattice filling is commensurate, super-counterflow can be observed\textsuperscript{2,4}. The two-component DSF density was also studied with mean field\textsuperscript{9,11} and quantum Monte Carlo (QMC) as was the three component case\textsuperscript{11}. Mean field gives a DSF density proportional to the square of the interspecies interaction for the two-component case leading to the conclusion that this effect is independent of the sign of the coupling. This would mean that for both, repulsive and attractive, inter-component interactions there are three contributions to the superflow: Those due to the two individual bosonic components and the DSF component. On the other hand, since bosons can be more easily cooled to very low temperatures, it was argued that pairing between fermions can be studied on optical lattices by considering two-component bosonic system with large intra-atomic repulsion, mimicking hard core bosons, and attractive inter-component interaction\textsuperscript{12}. It is well known that attracting fermions undergo pairing correlations: BCS-like for weak and tight binding (molecular) for strong attraction. Consequently, in this picture, all transport is expected to be superconducting (SC): There is no normal metallic transport when fermions are paired. This should imply the same behavior in the attractive bosonic case too, but this is not quite the picture emerging in the recent literature\textsuperscript{10,16,17}. While there is obvious consensus that when the attraction is strong enough, the bosons are tightly paired and transport is only via pair superfluidity (PSF), there is no consensus\textsuperscript{16} on the weakly attractive case. Mean field calculations\textsuperscript{9,11} show for weak inter-species coupling, the DSF in the repulsive case is equivalent to the PSF in the attractive case and that the corresponding SF densities are symmetric with respect to the interaction sign. For bosons with strong, but finite, intra-species repulsion in one dimension, renormalization group calculations\textsuperscript{16} argue that, for weak interaction, one needs a minimum attraction to form PSF and that PSF may co-exist with charge density wave (CDW).

We address these issues here and present QMC and DMRG results arguing that the balanced-population two-component boson system exhibits very different behavior for positive and negative interspecies interaction. Specifically, we show that while the repulsive case displays simultaneous DSF and individual component SF as
discussed in the literature\textsuperscript{13,14,15}, the attractive case has only pair SF for both hardcore and softcore boson systems with no single-component superfluidity. Using the hardcore boson/fermion analogy, these results also confirm the similarities in superfluid flow between fermion and boson systems. The systems we study are one-dimensional because (see below) the sizes needed to show pairing at weak attractive interaction are very large and cannot be reached in two dimensions with current algorithms and computers.

**Model and methods:** We study two-component Hubbard models on a one dimensional chain governed by the Hamiltonian $H = H_0 + H_{\text{int}}^F$ with

$$H_0 = -t \sum_{i,\sigma} \left( c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + \text{h.c.} \right)$$

$$H_{\text{int}}^F = U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

$$H_{\text{int}}^B = U \sum_i n_{i,\uparrow} n_{i,\downarrow} + U_0 \sum_{i,\sigma} n_{i,\sigma} (n_{i,\sigma} - 1),$$

(1)

where $F$ (B) refers to fermions (bosons). The creation (destruction) operator $c_{i,\sigma}^{\dagger}$ ($c_{i,\sigma}$) creates (destroys) fermions, soft- or hardcore bosons depending on the case being discussed. The number operator is $n_{i,\sigma}$. The two components are labeled by $\sigma = \uparrow, \downarrow$. We fix the energy scale by taking $t = 1$. Hardcore bosons and fermions are related by the Jordan-Wigner ( JW ) transformation and share many properties which we will delineate.

We studied these models, Eq. (1), using the ALPS library\textsuperscript{18} DMRG\textsuperscript{19,20} with open and periodic\textsuperscript{21} boundary conditions (OBC, PBC) and the stochastic Green function (SGF) QMC algorithm\textsuperscript{22,23} with PBC. The OBC DMRG calculations were done on lattices up to $L = 420$, whereas the PBC DMRG and QMC were done on $L$ up to 120. In all cases, we verified that the number of DMRG states and sweeps were sufficient for convergence to the ground state. To characterize the phases we calculate the single particle and pair Green functions, $G_{\sigma}(r)$ and $G_p(r)$,

$$G_{\sigma}(r) = \langle c_{i+r,\sigma}^{\dagger} c_{i,\sigma} \rangle,$$

$$G_p(r) = \langle P_{i+r,\uparrow} P_i \rangle,$$

$$P_i \equiv c_{i,\uparrow}^{\dagger} c_{i,\downarrow},$$

(2)

(3)

(4)

where $P_j$ is a pair annihilation operator at site $i$. Pair formation is signaled by power law decay of $G_p(r)$ concurrent with exponential decay of the single particle Green functions\textsuperscript{21,22}, $G_{\sigma}(r) \sim \exp(-r/\xi)$. It is important to note that the JW string factors cancel out when computing the pair Green function, meaning that fermionic and HCB pair correlations always exhibit the same behavior in any dimension. In addition, we compute the single particle charge gap\textsuperscript{26,27},

$$\Delta = E(N_\uparrow + 1, N_\downarrow) + E(N_\downarrow - 1, N_\uparrow) - 2E(N_\uparrow, N_\downarrow),$$

$$= E(N_\uparrow, N_\downarrow + 1) + E(N_\downarrow, N_\uparrow - 1) - 2E(N_\uparrow, N_\downarrow),$$

(5)

where $E(N_\uparrow, N_\downarrow)$ is the ground state energy with $N_\sigma (N_\downarrow)$ up (down) particles.

We probe transport via the $2 \times 2$ symmetric Drude weight tensor, $D$,

$$D_{\sigma\sigma'} = \frac{\pi L}{2t} \frac{\partial^2 E_0(\Phi_\sigma, \Phi_{\sigma'})}{\partial \Phi_\sigma \partial \Phi_{\sigma'}} \bigg|_{(\Phi_\sigma, \Phi_{\sigma'}) = (0, 0)}. $$

(6)

The phase twists $\Phi_\sigma$ are applied via the replacement $c_{n\sigma} \to e^{i \phi_\sigma} c_{n\sigma}$, where $\phi_\sigma = \Phi_\sigma / L$ is the phase gradient. This endows the hopping terms with a phase $\exp (i \phi_\sigma)$ (or its complex conjugate). The full tensor $D$ can be reconstructed by fitting the curvature of the ground state energy as a function of a phase $\Phi$ in the following four cases. The single particle weights are given by the diagonal, $D_{\sigma\sigma}$, calculated with $(\Phi_\uparrow, \Phi_\downarrow) = (\Phi, 0)$ or $(\Phi_\uparrow, \Phi_\downarrow) = (0, \Phi)$. The correlated weight corresponds to applying the same phase gradient on both components, $(\Phi_\uparrow, \Phi_\downarrow) = (\Phi, \Phi)$ giving: $D = D_C = D_{\uparrow\uparrow} + D_{\downarrow\downarrow} + D_{\uparrow\downarrow} + D_{\downarrow\uparrow}$. The anti-correlated weight is obtained by applying opposing gradients on the two components, $(\Phi_\uparrow, \Phi_\downarrow) = (\Phi, -\Phi)$, giving: $D^A = D_{\uparrow\downarrow} + D_{\downarrow\uparrow} - D_{\uparrow\uparrow} - D_{\downarrow\downarrow}$.

For bosonic systems these quantities probe superfluid transport and correspond to the variance of the winding numbers\textsuperscript{28,29} $W_\sigma$,

$$\rho_{\sigma} = \frac{L(W^2_\sigma)}{2t \beta} = D_{\sigma\sigma}$$

$$\rho^C = \frac{L(W^2_\uparrow + W^2_\downarrow)}{2t \beta} = D^C$$

$$\rho^A = \frac{L(W^2_\uparrow - W^2_\downarrow)}{2t \beta} = D^A,$$

(7)

(8)

(9)

where $\beta$ is the inverse temperature. This yields $D_{\downarrow\uparrow} = D_{\downarrow\uparrow} = \frac{L(W_\uparrow W_\downarrow)}{2t \beta}$. The off-diagonal term of $D$ and the cross-windings can be used to study directly the drag and pair SF densities. We calculate $D_{\sigma\sigma'}$ using DMRG and for the superfluid densities we use SGF QMC where windings can be measured directly.

**Results:** We first verify numerically Eqs. (7-9) are satisfied and that results from our QMC and DMRG are in agreement. The top panel of Fig.\textsuperscript{I} shows the anticorrelated and pair SF densities for fermions and HCB in the range $-5 \leq U < 5$. In addition, we show results for three $U$ values obtained from the Drude weight tensor using DMRG. We see that agreement is excellent confirming the coherence of our treatment of fermions and HCB using QMC and DMRG. The bottom panel of Fig.\textsuperscript{I} shows the QMC evolution of the anticorrelated and pair SF densities with system size for HCB (and equivalently for fermions) and exhibits some noteworthy features. When
FIG. 1. (Color online) (a): Anticorrelated and pair SF density for HCB and fermions using SGF QMC show excellent agreement. The plus and star (orange) symbols show DMRG results using the Drude weight tensor. (b) Finite size dependence of anticorrelated and pair SF densities for HCB.

FIG. 2. (Color online) The ratio of pair to single component SF density rises rapidly to unity for $U < 0$. The saturation ratio is reached more rapidly as the system size increases. Inset: The same ratio as a function of $L^{-1}$ for selected values of $U$. Even for the weakest attraction, $U = -1.4$, the ratio increases toward saturation as $L$ increases.

$U > 0$, the SF densities suffer very little from finite size effects. Also, the DSF $(L(W_+ W_-)/2\beta)$ is small and increases very slowly with $U$. The situation is different when $U < 0$. For large $|U|$, the anticorrelated SF density vanishes (indicating $(W_+ W_-) = (W_+^2) = (W_-^2)$) and the PSF density suffers very little finite size effects, indicating that only PSF is present. For small $|U|$, we observe large finite size effects. The anticorrelated SF density vanishes more rapidly for larger systems while the PSF density rises more rapidly. The latter effect suggests that, in the thermodynamic limit, for any $U < 0$, the system is in the PSF phase and all transport is via pair hopping. This, of course, is expected from the relation between fermions and HCB via the JW transformation but it emphasizes the importance of finite size effects for small $|U|$. Another important feature is the lack of symmetry between $U < 0$ and $U > 0$, a feature which persists for soft core bosons contrary to mean field results.

To elucidate the pair nature of SF when $U < 0$, Fig. 2 shows, for HCB, the ratio of pair to single species SF densities as a function of $U$. For $U > 0$, this ratio is small (less than 0.1 for $U \leq 5$) and insensitive to finite size effects. On the contrary, when $U < 0$, the ratio rises rapidly to unity, and more rapidly the larger the system. The inset shows this ratio as a function of $L^{-1}$ for four values of $U$. For $U = -2$, the ratio reaches unity for $L = 120$, but is much smaller for smaller $L$. For $U = -1.8, -1.6$, the ratio does not saturate for the attainable $L$, but it does rise sharply. For $U = -1.4$ the ratio remains small. However, the mapping to the fermion system requires this ratio to be unity for any $U < 0$. The reason it is not unity for weak attraction is that this is the regime of BCS pairing where the correlation length, $\xi$, between the pair constituents increases exponentially. When $\xi > L$, a false nonzero single particle SF density will be measured because the members of such a large pair can still wind around the system independently. DMRG allows access to larger systems (with OBC) than QMC, and so, we show in Fig. 3 DMRG results for the single particle and pair Green functions at $U = -1.75$ and $L = 420$. It is clear in this figure that the pair Green function decays as a power and that the
where $\rho$ is the particle density of each species. For $U_c < U < 0$, pairs do not form and the system is in a phase made of an equal mixture of two independent superfluids. For $U < U_c$, a PSF phase is established which may even co-exist with CDW. We investigated these claims using DMRG with $U_0 = 10$, and $\rho = 1/3$ and system sizes up to $L = 420$. Equation (10) then predicts $U_c = -2.4$. Our DMRG results for the one-body and pair Green functions, for soft bosons at $U = -1.75$, are presented in Fig. 3 and show clearly that pair correlations decay as a power law while one-body correlations decay faster (exponential). In Fig. 4 we show the decay length, $\xi_{\text{HCB}}$, down to $|U| = -1.5$ where the correlation function is still exponential, and $\xi_{\text{HCB}} \approx 100$. Even at this very small value, the system is still in the PSF phase whereas it is predicted to be a mixture of two independent SF. Note that, even though our results do not definitively exclude the possibility that the PSF phase does terminate at a much smaller but finite negative $U$, we see no evidence for this. This agrees with Ref. [12], where the overlap between the exact soft-core boson and HCB ground states was shown to be close to one and a smooth function of $U$.

**Conclusion:** In summary, we have shown that, for HCB (and fermions) in 1D optical lattice, a BCS-like quantum phase transition, in the BKT universality class [24], takes place as soon as an attractive interaction ($U < 0$) exists: the system is driven into a PSF phase where single particle transport is fully suppressed and superfluidity is due only to pairs. As we demonstrated, for $U < 0$ the BCS-like exponential growth of the one-body Green function decay length, $\xi_{\text{HCB}}$, has been widely overlooked leading to misinterpreted finite-size driven transport properties. This is in sharp contrast with the repulsive case ($U > 0$) where transport comprises both a single particle and a two body component (drag superfluid), i.e. where power-law decays are much less sensitive to finite size. We expect a similar pairing behavior to hold for higher dimensions, i.e. a BCS-like transition to pair superfluidity as soon as $U < 0$ for HCB, making finite size effects even more of a limiting issue for numerical simulations.

Finally, for soft bosons, our results show that down to rather weak attractive interaction, the transport properties are very similar to those of HCB and fermions. We emphasize that, if it exists, the phase made of two independent superfluids and no pairing, would be present only for a much narrower interaction range than predicted in Ref. [10]. A more thorough study of this problem is beyond the scope of this paper and would require both a much more extended computational effort and a revised renormalization group analysis.

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[1] A. F. Andreev and E. P. Bashkin, Zh. Eksp. Teor. Fiz. 69, 319 (1975).
[2] D. V. Fil and S. I. Shevchenko, Phys. Rev. A 72, 013616 (2005).
[3] J. Linder and A. Sudbø, Phys. Rev. A 79, 063610 (2009).
[4] P. P. Hofer, C. Bruder, and V. M. Stojanović, Phys. Rev. A 86, 033627 (2012).
[5] A. B. Kuklov and B. V. Svistunov, Phys. Rev. Lett. 90, 100401 (2003).
[6] V. M. Kaurov, A. B. Kuklov, and A. E. Meyerovich, Phys. Rev. Lett. 95, 090403 (2005).
[7] A. Kuklov, N. Prokofev, and B. Svistunov, Phys. Rev. Lett. 92, 200402 (2004).
[8] A. Kuklov, N. Prokofev, and B. Svistunov, Phys. Rev. Lett. 92, 050402 (2004).
[9] Yariv Yanay, Erich J Mueller, [arXiv:1209.2446]
[10] Karl Sellin and Egor Babaev, Phys. Rev. B 97, 094517 (2018).
[11] S. Hartman, E. Erlandsen, and A. Sudbø, Phys. Rev. B 98, 024512 (2018).
[12] B. Paredes and J. I. Cirac, Phys. Rev. Lett. 90, 150402 (2003).
[13] F. Zhan, J. Sabbatini, M. J. Davis, and I. P. McCulloch, Phys. Rev. A 90, 023630 (2014).
[14] G. Ceccarelli, J. Nespolo, A. Pelissetto, and E. Vicari, Phys. Rev. A 92, 043613 (2015).
[15] G. Ceccarelli, J. Nespolo, A. Pelissetto, and E. Vicari, Phys. Rev. A 93, 033647 (2016).
[16] A. Hu, L. Mathey, I. Danshita, E. Tiesinga, C. J. Williams, and C. W. Clark, Phys. Rev. A 80, 023619 (2009).
[17] A. Hu, L. Mathey, E. Tiesinga, I. Danshita, C. J. Williams, and C. W. Clark, Phys. Rev. A 84, 041609(R) (2011).
[18] B. Bauer et al., J. Stat. Mech. P05001 (2011).
[19] S. White, Phys. Rev. B 49, 8656 (1994).
[20] S. R. White, Phys. Rev. B 52, 10345 (1993).
[21] R. Mondaini, G. G. Batrouni, B. Grémaud, Phys. Rev. B 82, 155142 (2018).
[22] V. G. Rousseau, Phys. Rev. E 77, 056705 (2008).
[23] V. G. Rousseau, Phys. Rev. E 78, 056707 (2008).
[24] T. Giamarchi, “Quantum physics in one dimension”, (Oxford University Press, Oxford, 2004).
[25] E. Fradkin, “Quantum physics in one dimension”, (Cambridge University Press, Cambridge, UK, 2nd ed, 2013).
[26] J. F. Dodaro, H.-C. Jiang, and S. A. Kivelson, Phys. Rev. B 95, 155116 (2017).
[27] J. Jünemann, A. Piga, S.-J. Ran, M. Lewenstein, M. Rizzi, and A. Bermudez, Phys. Rev. X 7, 031057 (2017).
[28] E.L. Pollock and D.M. Ceperley, Phys. Rev. B 36, 8343 (1987).