Pairing and Pair Superfluid Density in One-Dimensional Two-Species Fermionic and Bosonic 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 a uniform, i.e., with no confining potential, 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.

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Introduction.—Multicomponent quantum systems have long attracted interest, whether bosonic, fermionic, or mixtures thereof. Andreev and Bashkin [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 increased with the experimental realization of trapped ultracold bosonic and fermionic atoms and mixtures of the two. In these systems, parameters 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 [2] and on optical lattices [3,4]. 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, supercounterflow can be observed [5–8]. The two- and three-component DSF densities were also studied with mean field [9–11] and quantum Monte Carlo (QMC). On the other hand, because bosons can be more easily cooled to very low temperatures, it was argued that pairing between fermions can be studied on optical lattices using a two-component bosonic system with large intra-atomic repulsion, mimicking hard-core bosons, and attractive intercomponent interaction [12]. It is well known that attracting fermions undergo pairing correlations: BCS-like for weak and tight binding (molecular) for strong attraction [13–23]. 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 [10,24,25]. Whereas there is obvious consensus that, for strong enough attraction, the bosons are tightly paired and transport is only via pair superfluidity (PSF), there is no consensus on the weakly attractive case. Mean field calculations [9–11] show that for weak interspecies 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. This would mean that for both repulsive and attractive interactions there are three contributions to the superflow: those due to the two individual bosonic components and to the DSF component. For bosons with strong but finite intraspecies repulsion in one dimension, renormalization group calculations [24] argue that, for weak interaction, one needs a minimum attraction to form PSF and that PSF may coexist with charge density wave (CDW).

We address these issues in this Letter 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 [1–3,10,11,26–28], the attractive case has only pair SF for both hard-core and soft-core boson systems with no single-component superfluidity. In other words, in the attractive case, transport takes place only via strongly or weakly paired particles, depending on the $|U|$. The single-particle Green's function decays exponentially, signifying an absence of single-particle transport; the pair Green's function decays as a power indicating quasi-long-range order, i.e., a critical phase in the Berezinskii-Kosterlitz-Thouless (BKT) universality class [29–33]. Using the analogy between fermions and hard-core bosons, these results confirm the similarities in SF flow between fermion and boson systems. We study one-dimensional systems because the sizes needed to exhibit pairing at weak attraction are very large and cannot be reached in two dimensions with current algorithms and computers. In addition, interest in one-dimensional superconductivity has sharply intensified as a result of a potentially wide range of applications, especially in quantum technologies, nanocircuits, single-photon detectors, etc. [34,35]. For these systems, it is crucial to have a clear understanding of their SF properties and the mechanisms that could disrupt them (temperature, defects…). Recent progress in understanding the impact of quantum phase slips was not based on actual pair formation but on simpler bosonic models [36–38]. From that viewpoint, this Letter addresses models that are more directly connected to conventional one-dimensional superconductivity.

Model and methods.—We study two-component Hubbard models on a one-dimensional chain governed by the $U(1)$ symmetric Hamiltonian $H = H_0 + H_{\text{int}}^{F/B}$:

$$H_0 = -t\sum_{i,\sigma}(c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}),$$
$$H_{\text{int}}^F = U\sum_i n_{i,\uparrow}n_{i,\downarrow},$$
$$H_{\text{int}}^B = U\sum_i n_{i,\uparrow}n_{i,\downarrow} + U_0\sum_{i,\sigma} n_{i,\sigma}(n_{i,\sigma}-1). \tag{1}$$

F (B) refers to fermions (bosons); the creation (destruction) operator $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (destroys) fermions and soft- or hard-core bosons; and the number operator is $n_{i,\sigma}$. The two components are labeled by $\sigma = \uparrow, \downarrow$. The interspecies interaction is $U > 0$ ($U < 0$) for the repulsive (attractive) cases. $U_0 > 0$ is the intraspecies repulsion and $U_0/t \to \infty$ gives the hard-core boson (HCB) limit. $t = 1$ fixes the energy scale. HCB and fermions are related by the Jordan-Wigner (JW) transformation [29,39] and share many properties that we will delineate. For fermions at incommensurate filling and $U = 0$, the renormalization group predicts a BKT-like transition between a gapless (metallic) phase for $U > 0$ to a spin gapped phase (BCS-like) for $U < 0$ [29].

We studied these models [Eq. (1)] using the ALPS library [40] DMRG [41,42] with open and periodic [43] boundary conditions (OBC, PBC) and the stochastic Green's function (SGF) QMC algorithm[44,45] with PBC. The OBC DMRG calculations were performed on lattices up to $L = 420$; the PBC DMRG and QMC were performed on L up to 120. In all cases, we verified that the numbers of DMRG states and sweeps were sufficient for convergence to the ground state. The various phases are characterized by the single-particle and pair Green's functions, $G_\sigma(r)$ and $G_p(r)$,

$$G_\sigma(r) = \langle c_{i+r,\sigma}^\dagger c_{i,\sigma}\rangle, \tag{2}$$

$$G_p(r) = \langle P_{i+r}^\dagger P_i\rangle, \tag{3}$$

$$P_i \equiv c_{i,\uparrow}c_{i,\downarrow}, \tag{4}$$

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 [29,46] of $G_\sigma(r) \sim \exp(-r/\xi)$. It is important to note that the JW string terms cancel for the pair Green's function, meaning that fermionic and HCB pair correlations always exhibit identical behavior in any dimension. In addition, we compute the single-particle charge gap [47,48],

$$\begin{aligned}\Delta &= E(N_\uparrow+1,N_\downarrow)+E(N_\uparrow-1,N_\downarrow)-2E(N_\uparrow,N_\downarrow)\\ &= E(N_\uparrow,N_\downarrow+1)+E(N_\uparrow,N_\downarrow-1)-2E(N_\uparrow,N_\downarrow),\end{aligned} \tag{5}$$

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

We probe transport via the 2×2 symmetric Drude weight tensor, $\mathbf{D}$,

$$\mathbf{D}_{\sigma\sigma'} = \frac{\pi L}{2t}\frac{\partial^2 E_0(\Phi_\sigma,\Phi_{\sigma'})}{\partial\Phi_\sigma\partial\Phi_{\sigma'}}\bigg|_{(\Phi_\sigma,\Phi_{\sigma'})=(0,0)}. \tag{6}$$

The phase twists Φ_σ are applied via the replacement $c_{n\sigma} \to e^{in\phi_\sigma}c_{n\sigma}$, 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 $\mathbf{D}$ can be reconstructed by fitting the curvature of the ground state energy as a function of a phase Φ 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 $D = D^{\text{C}} = D_{\uparrow\uparrow} + D_{\downarrow\downarrow} + D_{\uparrow\downarrow} + D_{\downarrow\uparrow}$. The anticorrelated weight is obtained by applying opposing gradients on the two components, $(\Phi_\uparrow, \Phi_\downarrow) = (\Phi, -\Phi)$, giving $D^{\mathrm{A}} = D_{\uparrow\uparrow} + D_{\downarrow\downarrow} - D_{\uparrow\downarrow} - D_{\downarrow\uparrow}$.

For bosonic systems, these quantities probe SF transport and correspond to the variance of the winding numbers [49,50] W_σ,

$$\rho_{s\sigma} = \frac{L\langle W_\sigma^2\rangle}{2t\beta} = \mathbf{D}_{\sigma\sigma}, \tag{7}$$

$$\rho_s^C = \frac{L\langle (W_\uparrow + W_\downarrow)^2\rangle}{2t\beta} = D^C, \tag{8}$$

$$\rho_s^A = \frac{L\langle (W_\uparrow - W_\downarrow)^2\rangle}{2t\beta} = D^A, \tag{9}$$

where β is the inverse temperature. This yields $D_{\downarrow\uparrow} = D_{\uparrow\downarrow} = L\langle W_\uparrow W_\downarrow\rangle/2t\beta$: the off-diagonal term of $\mathbf{D}$ and the cross-winding can be used to study directly the drag and pair SF densities. We calculate $\mathbf{D}_{\sigma\sigma'}$ using DMRG and for the SF densities we use SGF QMC, where windings can be measured directly.

Results.—We first verify Eqs. (7)–(9) numerically, and that our QMC and DMRG results are in agreement. The top panel of Fig. 1 shows the anticorrelated and PSF densities for fermions and HCB for $-5 \leq U < 5$. In addition, we show DMRG results for three U values obtained from the Drude weight tensor: agreement is excellent, confirming the coherence of our treatment of fermions and HCB using QMC and DMRG. The bottom panel of Fig. 1 shows the QMC evolution of the anticorrelated and PSF densities with system size for HCB (and equivalently for fermions) and exhibits some noteworthy features. For $U > 0$, the SF densities suffer very little from finite size effects, and the DSF ($L\langle W_\uparrow W_\downarrow\rangle/2\beta$) is small and increases very slowly with U. The situation is different when $U < 0$. For large $|U|$, the anticorrelated SF density vanishes (indicating $\langle W_\uparrow W_\downarrow\rangle = \langle W_\uparrow^2\rangle = \langle W_\downarrow^2\rangle$) 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 that persists for soft-core bosons, contrary to mean field results [9–11].

To elucidate the PSF nature 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. It is very well known that any finite attractive interaction between fermions triggers the

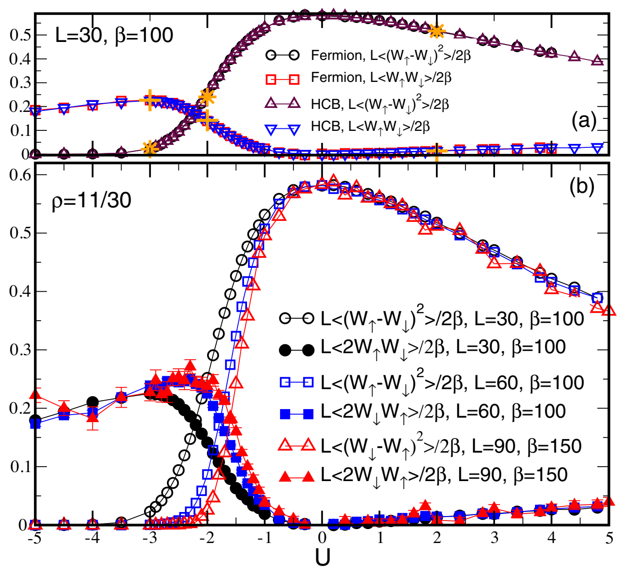

FIG. 1. (a) Anticorrelated and pair SF density for HCB and fermions using SGF QMC show excellent agreement. The plus and star (orange) symbols show DMRG results using the Drude weight tensor. (b) Finite size dependence of anticorrelated and pair SF densities for HCB.

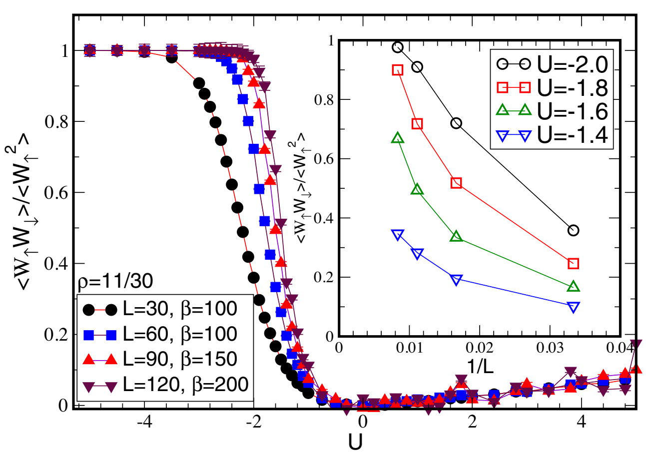

FIG. 2. The ratio of pair to single-component SF density rises rapidly to unity for $U < 0$. The saturation ratio is reached more rapidly as the system size increases. Inset: the same ratio as a function of L^{-1} for selected values of U. Even for the weakest attraction, $U = -1.4$, the ratio increases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

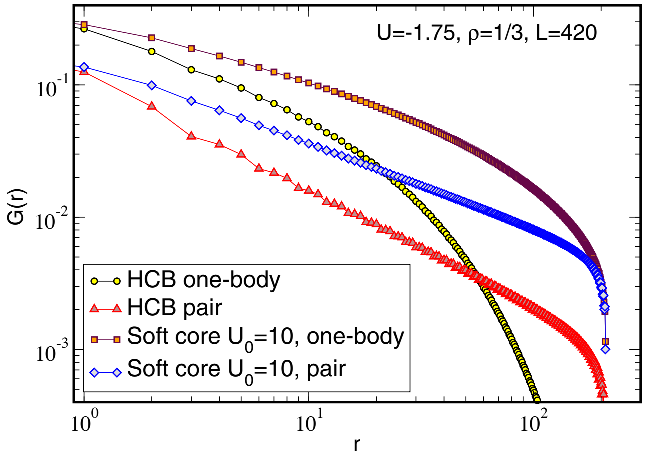

FIG. 3. Single-particle and pair Green's functions for HCB and soft-core bosons ($U_0 = 10$). Pair Green's functions decay as powers whereas the single-particle correlations decay exponentially for both HCB and soft-core bosons. $L = 420$ was necessary to expose the exponential decay for the soft-core case due to the much longer correlation length. For HCB, the power law exponent is slightly higher than unity, the value predicted at the transition [29].

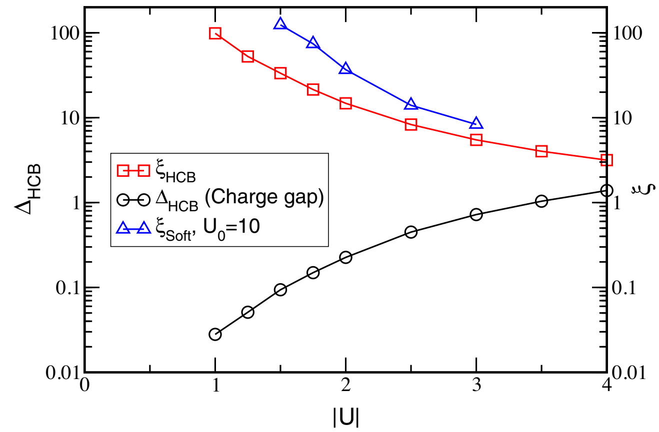

FIG. 4. Single-particle charge gap Δ_{HCB} [Eq. (5)] and Green's function decay length ξ_{HCB} for HCB as functions of the $|U|$, at fixed density $n_\uparrow = n_\downarrow = 1/3$. Because of BCS-like behavior at small $|U|$, ξ_{HCB} (Δ_{HCB}) diverges (vanishes) exponentially. For all $|U|$, the pair gap is always smaller than the numerical precision and is consistent with zero. For soft-core bosons at $U_0 = 10$, our results show that ξ exceeds 100 sites at $U = -1.5$, but the accuracy is limited by the numerics. Nevertheless, our results clearly emphasize that the system is still in a PSF phase for $|U|$ much smaller than predicted in Ref. [24]; see Eq. (10).

formation of Cooper pairs. Therefore, the mapping of HCB to the fermion system implies that this ratio is 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 ξ between the pair constituents increases exponentially. For $\xi > L$, 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's functions at $U = -1.75$ and $L = 420$. It is clear in this figure that the pair Green's function decays as a power and that the single-particle function decays exponentially. We note, however, that even though it is unambiguously clear from this figure that, at $U = -1.75$, only paired HCB participate in superflow, Fig. 2 shows that the ratio of pair to single-particle SF density is only 0.8 on a lattice with $L = 120$ sites. The system size needs to be greater than $L = 120$ to see the full effect of pairing at this interaction.

In Fig. 4 we show the growth (decay) of the single-particle correlation length ξ_{HCB} (charge gap, Δ_{HCB}) as $|U|$ gets smaller. We see that for HCB, when $U = -1$, the correlation length is already $\xi_{HCB} \approx 100$, necessitating much larger system size. We note that the pair gap (energy cost for adding or removing a pair, not shown in Fig. 4) is always smaller than the numerical precision, as expected for a gapless pair SF.

How these results might extend to soft-core bosons [finite U_0 in Eq. (1)] was studied [12] for large $|U_0|$, where they were shown to hold true. Lower values of $|U_0|$ are more difficult to study because of the exponential divergence of ξ. This was addressed [24,25] numerically and analytically with the renormalization group. It was shown that, below full filling, there is critical negative value of the interparticle attraction U, U_c needed to trigger pair formation,

$$\frac{U_c}{U_0} = -32\frac{t^2}{U_0^2}\sin^2(\pi\rho), \tag{10}$$

where ρ 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 SFs. For $U < U_c$, a PSF phase is established that may even coexist 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's 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). Figure 4 shows the decay length ξ_{Soft} down to $|U| = -1.5$, where the correlation function is still exponential, and $\xi_{Soft} \approx 100$. Even at this very small value, the system is still in the PSF phase whereas it is predicted to be [24] in a mixture of two independent SFs. 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 1 and a smooth function of U.

Conclusion.—We have shown with DMRG and QMC that two-species HCB and fermions in one-dimensional optical lattices exhibit identical transport properties; in particular, both systems exhibit the same PSF phase for $U < 0$ on the finite lattice sizes accessible to QMC and DMRG. Furthermore, it is well known for fermions that for any $U < 0$, Cooper pairs form and the system becomes superconducting even for infinitesimal U [13,14], and that, because of the $U(1)$ symmetry of the Hamiltonian, this transition is expected to be in the BKT universality class [29]. This, and our demonstration that the two-species HCB model behaves like the fermionic system, lead us to the conclusion that, as soon as an attractive interaction is present, HCB will also undergo a BKT transition to PSF where single-particle transport is suppressed and SF is due only to pairs. As we demonstrated, for $U < 0$ the BCS-like exponential growth of the one-body Green's function decay length ξ_{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 SF), 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.

For soft bosons, our results show that even at 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 SFs and no pairing would be present only for a much narrower interaction range than predicted in Ref. [24]. A more thorough study of this problem is beyond the scope of this Letter and would require both a much more extended computational effort and a revised renormalization group analysis.

Finally, as explained in the Introduction, one-dimensional nanowires have become crucial components in quantum technologies, as long as they remain perfectly superconducting. However, defects (or temperature) cause excitations leading to quantum phase slips and loss of SF. We expect similar behavior in our fermionic and bosonic Hubbard models. Consequently, cold atoms in optical lattices could serve as perfect theoretical and experimental test beds for probing the effect of phase slips on transport [37,38].

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