Exact Numerical Study of Pair Formation with Imbalanced Fermion Populations

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We present an exact quantum Monte Carlo study of the attractive one-dimensional Hubbard model with imbalanced fermion population. The pair-pair correlation function, which decays monotonically in the absence of polarization P, develops oscillations when P is nonzero, characteristic of Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase. The pair momentum distribution peaks at a momentum equal to the difference in the Fermi momenta. At strong coupling, the minority and majority momentum distributions are shown to be deformed, reflecting the presence of the other species and its Fermi surface. The FFLO oscillations survive the presence of a confining potential, and the local polarization at the trap center exhibits a marked dip, similar to that observed experimentally.

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Following the observation of Mott insulating transitions as the interaction strength is tuned [1], ultracold atoms trapped on optical lattices have been increasingly used to emulate the rich physics of strongly correlated condensed matter systems. One of the subtle phenomena being sought is the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase [2,3], in which an imbalance in the populations of up and down spin electrons leads to Cooper pair formation and Bose-Einstein condensation in states at nonzero momentum and to spatial inhomogeneities of the pairing and spin correlations. The observation of the FFLO phase in solids proved very difficult and was only achieved recently in heavy fermion systems [4].

Experiments, in which two hyperfine states of ultracold fermionic atoms play the role of up and down spins, have now reported the presence of pairing in the case of unequal populations [5,6]. Theoretical studies using mean field [7–16], effective Lagrangian [17], bosonization [18], and Bethe ansatz [19] are reported for the uniform system with extensions to the trapped system using the local density approximation. For the uniform case, the debate revolves on the details for the paired state: FFLO pairs forming with nonzero momentum vs breached pairing (BP) at zero momentum [15,16,20] and on the fragility of such phases. A distinguishing feature is the presence of spatial modulations (inhomogeneity) in the order parameter in the FFLO case, as opposed to coexistence of superfluid and normal components in a translationally invariant and isotropic state in the BP scenario. No general consensus has emerged on which pairing type dominates.

In this paper we report an exact quantum Monte Carlo study of pairing in one-dimensional fermion systems with population imbalance. We focus first on the homogeneous (untrapped) case since even here there is no agreement on the pairing mode. Our key result is that the FFLO phase is very robust and appears to be the dominant pairing mechanism. We show that the pair Green function exhibits oscillations characteristic of this phase, leading the pair momentum distribution function to peak at a momentum corresponding to the difference of the Fermi momenta of the individual species. In the last section, we consider the trapped system and how the basic FFLO phenomena survive the resulting density and polarization inhomogeneity. In addition, we show that at large $|U|$ the difference in density between the two species exhibits a deep minimum in the trap center in good agreement with experiments [5,6].

We first describe the model and the quantum Monte Carlo method we employed. The attractive Hubbard Hamiltonian is

$$\hat{\mathcal{H}} = -t\sum_{l\sigma}(c^\dagger_{l+1\sigma}c_{l\sigma} + c^\dagger_{l\sigma}c_{l+1\sigma}) + U\sum_l n_{l1}n_{l2} + V_T\sum_l l^2(n_{l1} + n_{l2}), \quad (1)$$

where $c^\dagger_{j\sigma}(c_{j\sigma})$ are fermion creation (destruction) operators on spatial site j with the fermionic species labeled by $\sigma = 1, 2$ and $n_{j\sigma} = c^\dagger_{j\sigma}c_{j\sigma}$ the corresponding number operator. We take the hopping parameter $t = 1$ to set the energy scale and attractive on-site interactions $U < 0$. V_T is the strength of the quadratic confining potential. All our results are for inverse temperature $\beta = 64$, so that $T = W/256$ with $W = 4t$ the bandwidth. We have verified that this yields ground state properties. We study a one-dimensional lattice with $L = 32$ sites and periodic boundary conditions, unless otherwise stated.

For our simulations, we use a continuous imaginary time canonical "worm" algorithm where the total number of particles is maintained strictly constant [21]. In this algorithm, two worms are propagated, one for each type of fermion, which allows the calculation of the real-space Green functions of the two fermionic species, G_σ, and also the pair Green function, G_{pair}, which are defined by

$$G_\sigma(l) = \langle c_{j+l\sigma} c^\dagger_{j\sigma} \rangle, \qquad G_{\text{pair}}(l) = \langle \Delta_{j+l} \Delta^\dagger_j \rangle \qquad \Delta_j = c_{j2} c_{j1}, \tag{2}$$

with Fourier transforms $n_\sigma(k)$ and $n_{\text{pair}}(k)$. We emphasize that this algorithm is exact: there are no approximations and the only errors are statistical (which are in all cases smaller than the symbol size). The polarization is given by $P = (N_2 - N_1)/(N_2 + N_1)$, where $N_1(N_2)$ is the minority (majority) particle numbers. The associated Fermi wave vectors are $k_{F\sigma} = 2\pi N_\sigma/L$. A typical run takes a day or two on a desktop computer.

We begin with the uniform system, $V_T = 0$. In one dimension, spin, charge, and pair correlations of the Hubbard Hamiltonian in the ground state decay algebraically with increasing separation, with smallest exponent characterizing the phases [22]. Here, with only an attractive on-site interaction, the dominant order is in the s-wave superconducting channel. In Fig. 1 we show the real-space pair correlation function $G_{\text{pair}}(l)$ for fixed $U = -8$ and different P. $G_{\text{pair}}(l)$ decays monotonically for $P = 0$ but develops clear oscillations for $P \neq 0$. These oscillations are characteristic of the FFLO state: The mismatch of the two Fermi surfaces leads to pairing at nonzero center of mass momentum and, consequently, spatially inhomogeneous regions in which the pairing amplitude oscillates. The larger the Fermi surface mismatch, i.e., the larger the P, the larger the center of mass momentum and the smaller the period, as seen in Fig. 1. The modulations in $G_{\text{pair}}(l)$ follow the Larkin-Ovchinnikov [3] (LO) form where the order parameter is modulated with a $\cos(qr)$ as a function of position r with $q = \pm|k_{F1} - k_{F2}|$. The period, T, of the oscillations is given by $T = 2\pi/|q|$ as can be seen easily in Fig. 1.

To put the FFLO behavior in better context, we begin in Fig. 2 with $n_\sigma(k)$ and $n_{\text{pair}}(k)$ for the unpolarized case. At weak coupling, $U = -2$, the fermion momentum distribution function, $n_1(k) = n_2(k)$, has a sharp Fermi surface which is then increasingly rounded as $|U|$ increases. In all cases n_σ is a monotonic function of k. Meanwhile the pair momentum distribution function, $n_{\text{pair}}(k)$, has a peak at $k = 0$ which grows with $|U|$: the pairs have zero momentum and become more tightly bound and numerous the larger the on-site attraction.

When the system is polarized, it is thought to develop either pairs with nonzero momentum via the FFLO mechanism or zero momentum pairs via the BP mechanism [15,16,20]. We show in Fig. 3 the single particle and pair momentum distributions for $N_1 = 7$, $N_2 = 9$ ($P = 0.125$) with $U = -4$ and $U = -10$ on systems with $L = 32$ and $L = 96$ sites. We note the following features: (a) in both cases, $n_{\text{pair}}(k)$ peaks at $\pm|k_{F1} - k_{F2}|$ (we show only $k > 0$ since the figure is symmetric), (b) the height of the peak increases with increasing $|U|$, (c) in both cases, the Fermi surfaces for the minority and majority populations are much more sharply defined than their $P = 0$ counterparts at the same $|U|$. Another striking feature is the behavior of $n_2(k)$. For $U = -4$, $n_2(k)$ displays a dip at $k = 0.39 < k_{F2}$ which deepens as $|U|$ increases and spreads to $k = 0$: for $U = -10$, we see that $n_2(k \leq 0.59) \approx 0.54$ but then rises to $n_2(0.59 < k \leq 0.78) \approx 0.64$ before it drops at the Fermi surface. This remarkable feature, in which the momentum distribution can increase as k increases, is very robust for large negative $|U|$ and is not a finite size effect. Indeed, the physical origin of the dip is the suppression of the majority spin Fermi function by scattering off the minority species, which occurs preferentially for $k < K_{F1}$.

Similar behavior in the momentum distribution has been seen in mean field both for FFLO and BP in Ref. [16] where the Fulde-Ferrell (FF) single plane wave ansatz, $\Delta(r)e^{iqr}$, was used. In the BP case, $n_2(k)$ is symmetric around $k = 0$, whereas in the FFLO case $n_2(k)$ is asymmetric. It is likely that the LO ansatz with cosine modulation due to the superposition of two plane waves with opposite wave vectors will lead to a symmetric result for $n_2(k)$ in the FFLO state. However, there is no ambiguity in the pair momentum distribution, $n_{\text{pair}}(k)$: its peak lies at $k_{\text{peak}} = \pm|k_{F1} - k_{F2}|$ as is seen in Fig. 3. Furthermore, this peak starts to form at $k \neq 0$ even for the smallest values of $|U|$ we have examined. For example, for the case of Fig. 3, it is present at $U = -0.5$.

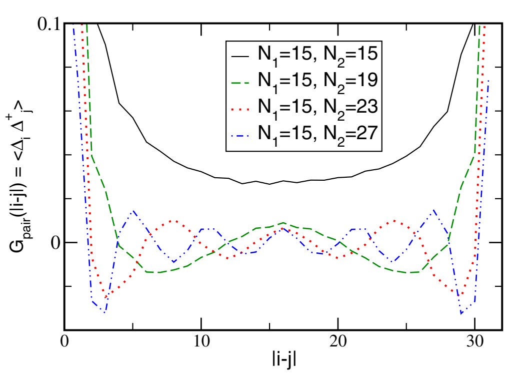

FIG. 1 (color online). The pair Green function $G_{\text{pair}}(|i - j|)$ for $N_1 = 15$ and $N_2 = 15$, 19, 23, 27 (polarizations $P = 0$, 0.118, 0.211, and 0.286) and $U = -8$.

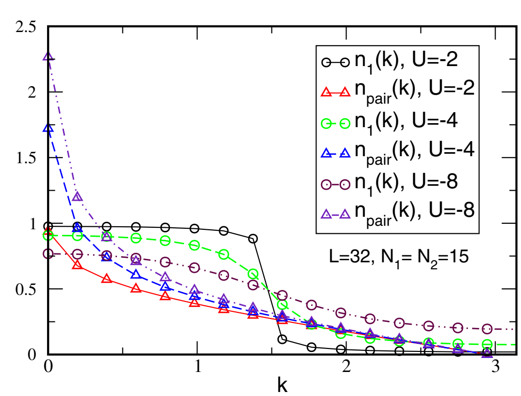

FIG. 2 (color online). $n_1(k)$ and $n_{\text{pair}}(k)$ for the case of $N_1 = N_2 = 15$ and $L = 32$, $\beta = 64$, $U = -2, -4, -8$. Here $P = 0$, so $n_1(k) = n_2(k)$.

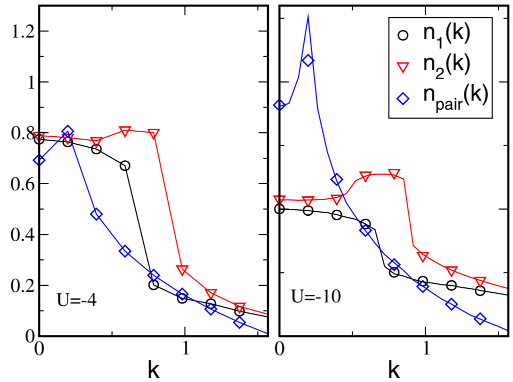

FIG. 3 (color online). Left: symbols and lines are for $U = -4$, $N_1 = 7$, $N_2 = 9$, $L = 32$, $\beta = 64$. Right: symbols are the same as left panel except $U = -10$; lines are for $L = 96$, $N_1 = 21$, $N_2 = 27$, and $\beta = 192$. Finite size effects are negligible, except for a sharper quasicondensate peak which is expected on larger lattices.

Additional insight on the pairing is obtained from the energetics. In Fig. 4 we show the kinetic energy (KE) per site for the minority and majority populations, $\langle c^\dagger_{l+1\sigma} c_{l\sigma}\rangle$, and for the pairs, $\langle \Delta_{l+1}\Delta^\dagger_l\rangle$. We also show the subtracted pair KE/site ($\langle \Delta_{l+1}\Delta^\dagger_l\rangle - \langle c^\dagger_{l1} c_{l1}\rangle\langle c^\dagger_{l2} c_{l2}\rangle$) to emphasize the contribution from pairing. We see that as $|U|$ increases, the single fermion kinetic energies decrease (in absolute value) while the pair KE increases: more and more of the fermion hopping is performed in pairs. We also see clear crossover behavior in the KE curves (change in the sign of the curvature) as $|U|$ is increased, which can be understood by examining the double occupancy, $\langle n_{i1}n_{i2}\rangle$. Clearly, $\langle n_{i1}n_{i2}\rangle$ lies between N_1N_2/L^2 at $U = 0$ (no pairing) and N_1/L at very large negative U (maximum pairing). When pairing is saturated, the system is made of N_1 tightly bound pairs and a gas of $N_2 - N_1$ unpaired fermions. The crossover in the KE appears to take place as the number of tightly bound pairs most rapidly approaches its saturation value at $U \approx -2.5$. We emphasize that for all values of U, the peak in $n_{\rm pair}$ is at $k_{\rm peak} \neq 0$ when $P \neq 0$.

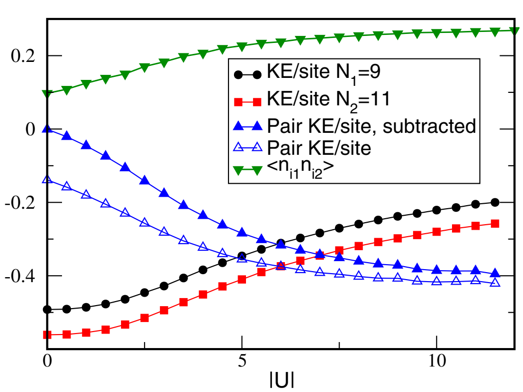

FIG. 4 (color online). Kinetic energy/site and the "double occupancy" $\langle n_{i1}n_{i2}\rangle$ versus $|U|$ for $L = 32$ and $\beta = 64$.

To underscore the robustness of FFLO pairing, we show $n_{\rm pair}(k)$ in Fig. 5 at $U = -9$ for several polarizations. The curves clearly show a peak at $k_{\rm peak} \neq 0$, which, as is seen in the inset, corresponds to $|k_{F1} - k_{F2}|$. It is striking that even at the largest polarizations considered, corresponding to $N_1 = 15$ and $N_2 = 31$, FFLO pairing is still present as seen in the $n_{\rm pair}(k)$ peak. For these parameters, we have not found the Clogston-Chandrasekhar limit [23] in which extreme polarization completely destroys the superconducting state. It is possible that going to much lower N_1 can reach it. Similar density matrix renormalization group (DMRG) results concerning FFLO pairing dominance and the Clogston limit have very recently been reported [24].

Several measurements have been reported on spin imbalanced cold atom systems [5,6] confined in three-dimensional, but highly elongated, traps. In these experiments, the effect of the confining potential is critical to the results. We now apply a trap, $V_T \neq 0$, in our simulations and discuss its effect on the FFLO pairing state. It is clear that the presence of the majority species in the trap center, combined with the attractive interaction, will lead to increased localization of the minority species in the center. Experiments [5,6] show additional interesting features: this localization tendency is so marked that the local density difference $n_{i2} - n_{i1}$ vanishes in an extended region about the trap center. One recent DMRG calculation [25] observes both the FFLO state and the squeezing of the minority population, but their local density difference is maximal at the trap center. More precisely, there is an extended flat region of constant local polarization near the center, which then falls off as the distance increases. The constancy of this polarization is reflected in the fact that the period of the FFLO oscillations is uniform throughout the central region.

A second DMRG treatment [26] studying several densities and polarizations, low and high, also gives evidence

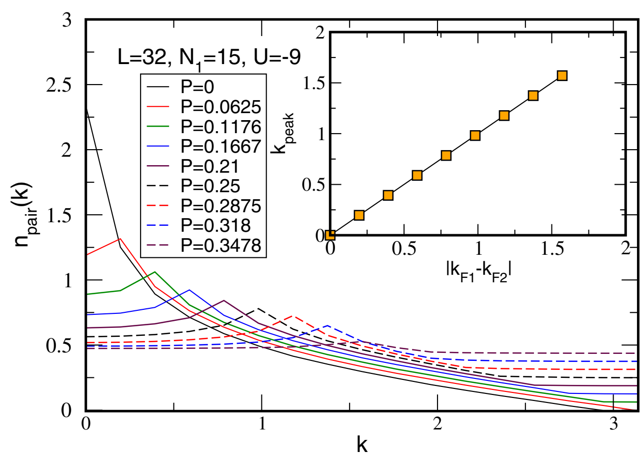

FIG. 5 (color online). $n_{\rm pair}(k)$ for several values of the polarization showing the FFLO peak going to higher values of $k_{\rm peak}$ as $|k_{F1} - k_{F2}|$ increases. The inset shows the position of the peak versus $|k_{F1} - k_{F2}|$.

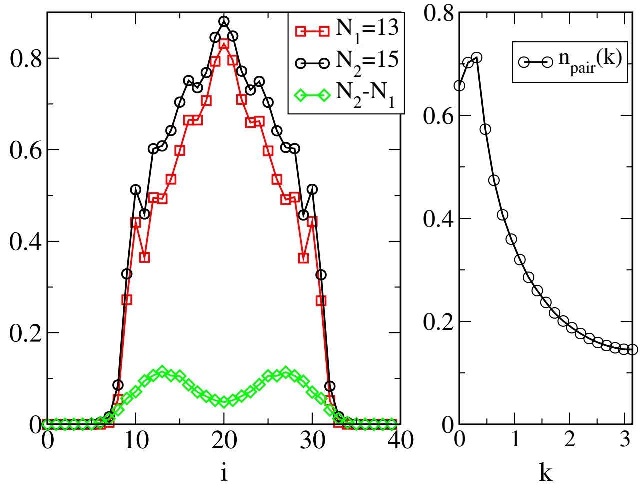

FIG. 6 (color online). Left: density profiles for the minority and majority populations in a trap $V_T = 0.005$, $L = 40$, $U = -10$, $\beta = 64$. The phase in the trap center is not a fully packed Fock state, yet the difference in the local density still exhibits a deep minimum. Right: the Fourier transform $n_{\text{pair}}(k)$ of the pair correlation function.

for an FFLO phase. However, zero density difference in the trap center is reported only for the case of a Fock state of sites which are fully occupied with $n_{i1} = n_{i2} = 1$. This leads to a vanishing local polarization, but does not support superconductivity (at any wave vector) since the particles cannot move. At larger global polarization the Fock state melts and the minimum in local polarization is nonvanishing at the trap center, but the state there is metallic rather than superconducting, since the sites are still fully occupied in the majority channel.

In Fig. 6 we show that a marked minimum in the density difference is present even when the trap center is superfluid, with both $n_{i1} < 1$ and $n_{i2} < 1$, as in the experimental situation. The figure also shows a peak in $n_{\text{pair}}(k)$ at nonzero k, demonstrating that pairing occurs and, furthermore, that this superfluid is of the FFLO variety, as expected from the nonzero local polarization, p_i. At the trap center, $p_i = n_{i1} - n_{i2} = 0.049$, which would lead to FFLO pairing at $k_a = 0.31$ in the uniform case. Towards the edge of the central polarization minimum, the maximal $p_i = 0.115$, with an associated $k_b = 0.72$. The observed peak in $n_{\text{pair}}(k)$ lies very close to k_a and is determined by the lower polarization region.

To conclude, we studied the $d = 1$ attractive Hubbard model with imbalanced populations for a range of P and U with and without a trapping potential. In the absence of a trap, we presented results for pair Green functions, single particle and pair momentum distributions, and kinetic and interaction energies. Our results show that FFLO pairing is robust from very small values of $|U|$ all the way to saturation at very large $|U|$ and for a wide range of P. We found no values of U and P for which BP dominates over FFLO: the maximum of $n_{\text{pair}}(k)$ is always at $k_{\text{peak}} = \pm|k_{F1} - k_{F2}|$. We have also shown that at large $|U|$, $n_\sigma(k)$ of the majority populations is not monotonic. Finally, these features are robust to the spatial inhomogeneities induced by the presence of a trap.

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