



## Superconductivity and charge order of confined Fermi systems

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The low-temperature properties of the two-dimensional attractive Hubbard model are strongly influenced by the fermion density. Away from half-filling, there is a finite-temperature transition to a phase with  $s$ -wave pairing order. However,  $T_c$  is suppressed to zero at half-filling, where long-range charge-density-wave order also appears, degenerate with superconductivity. This paper presents determinant quantum Monte Carlo simulations of the attractive Hubbard model in the presence of a confining potential  $V_{\text{trap}}$  which makes the fermion density  $\rho$  inhomogeneous across the lattice. Pair correlations are shown to be large at low temperatures in regions of the trapped system with incommensurate filling, and to exhibit a minimum as the local density  $\rho(i)$  passes through one fermion per site. In this ring of  $\rho(i) = 1$ , charge order is enhanced. A comparison is made between treating  $V_{\text{trap}}$  within the local-density approximation (LDA) and in an *ab initio* manner. It is argued that certain sharp features of the LDA result at integer filling do not survive the proximity of doped sites. The critical temperature of confined systems of fixed characteristic density is estimated.

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### I. INTRODUCTION

Studies of the interplay of spatial inhomogeneity and superconductivity have a long history. A seminal early result was Anderson's realization<sup>1</sup> that although the breaking of translation invariance by disorder renders momentum no longer a good quantum number, pairing still occurs between appropriately chosen (time reversed) states. Numerical studies within the Bogoliubov-de Gennes approximation,<sup>2,3</sup> quantum Monte Carlo (QMC),<sup>4</sup> and other approaches have quantified the magnitude of disorder which superconductivity can withstand.<sup>5</sup> In these studies, and the granular superconducting materials they model,<sup>6</sup> regions of pairing order coexist with normal, or insulating, phases. Superconductivity can be destroyed by various mechanisms, including phase fluctuations between the order parameter on different islands where Cooper pairs exist,<sup>7</sup> or breaking of the Cooper pairs themselves.<sup>8</sup> The dominant mechanism determines the appropriate modeling, e.g., a description within the disordered boson<sup>9</sup> or fermion Hubbard Hamiltonians, or "phase-only" descriptions with the XY model and its variants.<sup>10</sup>

Recently, experiments on ultracold atoms have provided a rather different realization of inhomogeneity in the form of a smoothly varying confining potential which produces a system with a radial density profile, maximal at the trap center and falling off to zero at the periphery.<sup>11</sup> Much attention has focused on repulsively interacting bosons and fermions.<sup>12,13</sup> In this case, a Mott insulator may coexist with superfluid or normal phases. For fermions, the Mott insulator also exhibits antiferromagnetic correlations at very low temperatures. At present, experimentally accessible temperatures for fermionic systems are such that a degenerate Fermi gas has been observed,<sup>14</sup> along with signatures of the Mott phase.<sup>15,16</sup> The ultimate objective is insight into the ground-state physics of the repulsive Hubbard model (RHM), and, in particular, the

fundamental issue of  $d$ -wave superconducting order and its interplay with antiferromagnetism.<sup>17</sup>

This goal for repulsive fermions awaits the attainment of lower experimental temperatures. In the interim, it is useful to perform careful studies of attractive systems. This case is not only of interest in its own right, but also QMC simulations can often attain lower temperatures for attractive models, and thus can track experiments closer to transitions into ordered phases.

The focus of the present paper is the description of the behavior of attractively interacting fermions in a two-dimensional confining potential. Some of the issues are similar to the repulsive case, in particular, the coexistence of phases as the density varies across the trap.<sup>18</sup> However, the attractive case has several important distinctions, specifically the existence of known finite-temperature phase transitions in two dimensions. In addition, in the repulsive case there is a broad range of chemical potentials  $\mu$  which fall within the "Mott gap" and for which the fermion density  $\rho = 1$ . That is, the compressibility  $\kappa = \partial\rho/\partial\mu = 0$  at  $\rho = 1$ . For the confined system, this implies an extended region of commensurate density, spatial sites which have a value of the local confining potential which falls within the Mott gap. In the attractive case, the compressibility is finite ( $\kappa \neq 0$ ) at commensurate density. As a consequence, the region of half-filling is a truly one-dimensional ring as opposed to an annulus of finite thickness.

A key result of this work is that the unique features of charge-density-wave physics at the single value of chemical potential which gives commensurate filling do not survive coupling to neighbors of incommensurate density. Thus the correlations which appear in a homogeneous system with commensurate filling are never achieved in a trap; the local-density approximation (LDA), in which the behavior of each site in a confining potential is assumed to be that of a homogeneous system with global density matching the local filling, breaks down at that point.

This paper is organized as follows: In the next section we describe the specific Hamiltonian, the attractive Hubbard model (AHM), and aspects of the computational methodology, determinant quantum Monte Carlo (DQMC), which will be used. Results are then presented within the LDA as well as from direct simulations of confined systems, and the two approaches are compared. Next, we present a finite-size extrapolation using data from systems of different sizes at constant characteristic density, and estimate the critical temperature of the confined AHM. A concluding section summarizes the results and indicates some remaining open questions.

Studies of the AHM with inhomogeneity have been performed with variational Monte Carlo,<sup>19</sup> Bogoliubov–de Gennes,<sup>20,21</sup> and Gutzwiller approaches.<sup>22,23</sup> Of particular relevance here is work within dynamical mean-field theory (DMFT) and a two-site impurity solver,<sup>24</sup> which suggested that the half-filled physics is stabilized by a confining potential, and that an extended supersolid phase of commensurate density exists in a trap.

## II. MODELS AND COMPUTATIONAL APPROACH

The attractive Hubbard Hamiltonian, in the presence of a confining potential, reads

$$\hat{H} = -t \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) - |U| \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) - \sum_i \{\mu - V_{\text{trap}} |i|^2\} (n_{i\uparrow} + n_{i\downarrow}). \quad (1)$$

Here  $c_{i\sigma}^\dagger$  ( $c_{i\sigma}$ ) are creation (destruction) operators at spatial site  $i$  for two different species of fermions  $\sigma$ . We choose the center of the trap to be at a plaquette center and set the origin there, so that the coordinates  $i_x$  and  $i_y$  take half-integer values. In the condensed-matter context,  $\sigma = \pm \frac{1}{2}$  is the electron spin. For cold atoms,  $\sigma$  labels two hyperfine states. We will consider the case of square lattices of linear size  $L$ . The hopping parameter  $t$  can be tuned by changing the optical lattice depth;<sup>25</sup> in the following,  $t = 1$  is chosen to set the scale of energy. The sum  $\sum_{\langle ij \rangle}$  is over all near-neighbor pairs of sites, and  $\sum_i$  is over all sites. The on-site attraction  $|U|$  can be tuned through the application of a magnetic field via a Feshbach resonance. The chemical potential  $\mu$  is set to get the desired number of particles  $N$ . Finally,  $V_{\text{trap}}$  is the trap curvature which determines the strength of the confining potential.

In DQMC,<sup>26</sup> the partition function  $Z = \text{Tr} e^{-\beta \hat{H}}$  is written as a path integral by discretizing the inverse temperature  $\beta$  into  $M$  intervals of size  $\Delta\tau = \beta/M$ . The Trotter approximation<sup>27</sup>  $e^{-\Delta\tau \hat{H}} \simeq e^{-\Delta\tau \hat{K}} e^{-\Delta\tau \hat{V}}$  isolates the quartic terms (involving the interaction  $U$ ) in  $\hat{H}$ , and a discrete Hubbard-Stratonovich field<sup>28</sup> decouples  $e^{-\Delta\tau \hat{V}}$  so that only quadratic terms in the fermion operators appear. When the trace over fermion operators is done,  $Z$  is expressed as a sum over the different field configurations with a weight which is the product of two determinants (one for each value of  $\sigma$ ) of matrices with dimension  $L^2 \times L^2$  given by the number of lattice sites. In the case of attractive  $U$ , because the two species couple to the Hubbard-Stratonovich field with the same sign, the two

determinants are identical and there is no sign problem.<sup>29</sup> This allows us to study confined systems down to arbitrarily low temperatures, unlike the repulsive model where the largest  $\beta$  accessible is  $\beta \simeq 3\text{--}4$  for confined systems with  $U = 4\text{--}8$ .<sup>18</sup>

The observables which will be the focus of this paper are the  $s$ -wave pairing and charge-density-wave (CDW) correlation functions,

$$c_{\text{pair}}(\mathbf{i}, \mathbf{j}) = \langle \Delta_{\mathbf{i}+\mathbf{j}} \Delta_{\mathbf{i}}^\dagger \rangle, \quad (2)$$

$$c_{\text{charge}}(\mathbf{i}, \mathbf{j}) = \langle n_{\mathbf{i}+\mathbf{j}} n_{\mathbf{i}} \rangle - \langle n_{\mathbf{i}+\mathbf{j}} \rangle \langle n_{\mathbf{i}} \rangle,$$

where  $\Delta_{\mathbf{i}}^\dagger = c_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{i}\downarrow}^\dagger$  creates a *pair* of fermions on site  $\mathbf{i}$  and  $n_{\mathbf{i}} = n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow}$  counts the fermions on site  $\mathbf{i}$ . Notice that these depend on  $\mathbf{i}$  and not just on the separation  $\mathbf{j}$ . We also define the associated structure factors

$$P_S = \sum_{ij} c_{\text{pair}}(\mathbf{i}, \mathbf{j}), \quad (3)$$

$$S_{\text{CDW}} = \sum_{ij} (-1)^j c_{\text{charge}}(\mathbf{i}, \mathbf{j}).$$

In addition, we study the local quantities

$$\rho(\mathbf{i}) = \langle n_{\mathbf{i}\uparrow} \rangle + \langle n_{\mathbf{i}\downarrow} \rangle, \quad (4)$$

$$t(\mathbf{i}) = \frac{1}{2} \sum_j^{(ij)} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}),$$

$$D(\mathbf{i}) = \langle n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \rangle - \langle n_{\mathbf{i}\uparrow} \rangle \langle n_{\mathbf{i}\downarrow} \rangle;$$

the density  $\rho(\mathbf{i})$  has already been used;  $t(\mathbf{i})$  is the kinetic energy<sup>30</sup> associated with the bonds of site  $\mathbf{i}$ ; and  $D(\mathbf{i})$  is the double occupancy with the trivial density dependence subtracted.

Before proceeding with the confined case, it is useful to review the properties of the translationally invariant case,  $V_{\text{trap}} = 0$ . In two dimensions, it is known that the half-filled attractive Hubbard Hamiltonian has combined long-range CDW and  $s$ -wave pairing order in its ground state, and is unordered at nonzero temperature.<sup>31</sup> When doped, the symmetry between charge and pairing is broken, and a Kosterlitz-Thouless (KT) transition to a quasi-long-range ordered superfluid phase occurs at finite temperature. Many numerical and analytical studies have been performed.<sup>32</sup> The transition temperature  $T_c$  rises rapidly as  $\mu$  is made nonzero and reaches a maximum value of  $T_c \simeq \frac{1}{10}$  for a wide range of fillings  $0.5 < \rho < 0.9$ .<sup>33</sup> The effect of inhomogeneities in the interaction strength has also been explored.<sup>3</sup>

Consideration of the ‘‘asymmetric’’ particle-hole (PH) transformation helps clarify these assertions. On a bipartite lattice, when the down-spin operators in the AHM [Eq. (1)] are mapped with

$$c_{i\downarrow} \leftrightarrow (-1)^i c_{i\downarrow}^\dagger, \quad (5)$$

the kinetic energy is unchanged, but the interaction term changes sign, so that the AHM maps onto the RHM [the phase factor  $(-1)^i$  is understood to take the values  $\pm 1$  on alternating sublattices]. This PH symmetry provides a simple argument that the two-dimensional half-filled AHM can have long-range order (LRO) only at  $T = 0$ , like the RHM.

QMC simulations have shown that the ground state of the half-filled two-dimensional uniform RHM is magnetically ordered.<sup>28</sup> PH symmetry then implies that CDW and pair order occur simultaneously in the  $T = 0$  half-filled AHM. To see this, note that the  $z$  component of spin  $n_{i\uparrow} - n_{i\downarrow}$  in the RHM maps onto the charge  $n_{i\uparrow} + n_{i\downarrow}$  in the AHM, so that magnetic LRO in the  $z$  direction of the RHM corresponds to CDW order of the AHM. Similarly, magnetic order in the  $xy$  plane maps onto  $s$ -wave pairing order. The degeneracy of the  $z$  and  $xy$  magnetic order in the repulsive model implies that CDW and pair order occur simultaneously in the half-filled attractive case.

A final consequence of PH symmetry is the explanation of the occurrence of pairing order (and the absence of CDW order) at finite temperature in the doped AHM. When doped,  $\mu$  is nonzero. Under the PH transformation of Eq. (5), the chemical potential term  $\mu(n_{i\uparrow} + n_{i\downarrow})$  in the AHM becomes a Zeeman field  $B(n_{i\uparrow} - n_{i\downarrow})$  in the RHM ( $B$  has the same numerical value as  $\mu$ ). Because the order in the RHM is antiferromagnetic, a uniform field in the  $z$  direction makes it energetically favorable for spins to lie in the  $xy$  plane, since then they can tilt out of the plane and pick up field energy without costing as much exchange energy. This lowering of symmetry from three to two components makes possible a finite-temperature Kosterlitz-Thouless transition in two dimensions. The  $xy$  magnetic order which exists in the RHM then maps to  $s$ -wave pair order in the AHM.

### III. CORRELATIONS AND THE LOCAL-DENSITY APPROXIMATION

We begin by showing the density profile in Fig. 1, along with the local kinetic energy and the double occupancy. Results are given both from the LDA and from a trapped  $30 \times 30$  system with  $N = 564.1 \pm 0.4$  particles. These two approaches yield results in very good agreement for  $\rho(i)$ ,  $t(i)$ , and  $D(i)$ . An important point is the absence of a density plateau at  $\rho = 1$ , in accordance with results in the LDA, and also with a particle-hole symmetry argument which identifies the compressibility  $\kappa = d\rho/d\mu$  of the AHM with the uniform magnetic susceptibility  $\chi = dM/dB$  of the RHM, which is known to be nonzero at zero external field; thus, as noted above, the AHM has finite compressibility at integer filling, and there is no Mott plateau at half-filling.

This true one dimensionality of the  $\rho(i) = 1$  ring makes the formation of long-range CDW order in the AHM much less robust than the antiferromagnetic order which can occur on the quasi-two-dimensional Mott annulus of integer filling that occurs in the RHM.

A related difference to the RHM is seen in the kinetic energy, which shows a maximum at half-filling in Fig. 1, where in the RHM the Mott phase would lead to localization and a minimum of the kinetic energy. This behavior is best understood by applying the asymmetric PH transformation. The corresponding RHM is uniformly half-filled and subject to a perpendicular Zeeman field  $B_i$  that varies radially and goes through zero at those sites  $i$  that had  $\rho(i) = 1$  in the original, attractive model. Away from the  $B = 0$  region, the system gets increasingly spin polarized and thereby makes Pauli exclusion more effective in hindering fermion mobility.

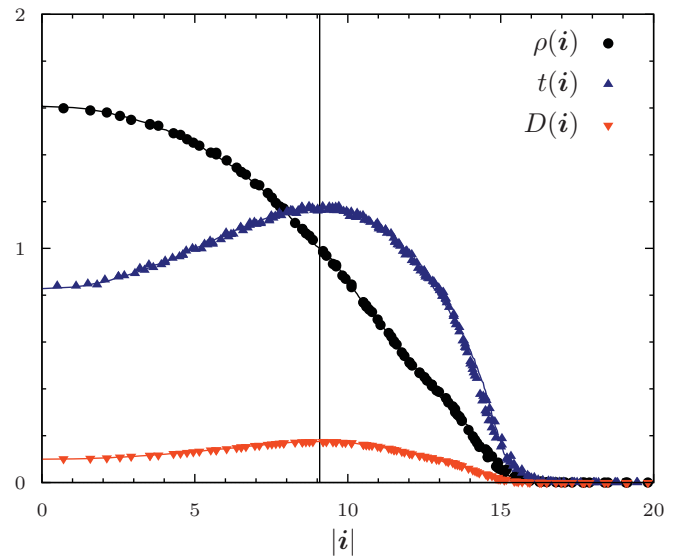


FIG. 1. (Color online) Fermion density  $\rho$ , kinetic energy  $t$ , and double occupancy  $D$  as a function of distance  $|i|$  from the trap center, with  $N = 564$  particles,  $U = 6$ ,  $V_{\text{trap}} = 0.0097$ , and  $\mu = 0.8$  at  $\beta = 9$ . The solid line shows the LDA result; in this case, near perfect agreement is found between the true trapped system and the LDA. Note that, in contrast to the RHM, there is no plateau at half-filling (marked by the vertical line), which corresponds to the absence of a Mott gap in the homogeneous model. Error bars are smaller than the symbols.

One therefore expects a maximum in both  $t(i)$  and  $D(i)$  when the site  $i$  belongs to the  $B_i = 0$  region. As these quantities are unchanged by the PH transformation, this last statement translates *verbatim* to the AHM.

Next, Fig. 2 shows the near neighbor  $c_{\text{pair}}(i, (\frac{1}{0}))$  and next-near neighbor  $c_{\text{pair}}(i, (\frac{1}{1}))$   $s$ -wave pairing correlators both in the LDA and the  $30 \times 30$  system. In the LDA, both functions dip at  $r = \sqrt{\mu/V_{\text{trap}}}$ , where the local density  $\rho(i) = 1$ , as do the corresponding farthest-neighbor correlators. Figure 3 shows the density correlators  $c_{\text{charge}}(i, (\frac{1}{0}))$  and  $|c_{\text{charge}}(i, (\frac{1}{1}))|$  which in the LDA peak as the system crosses through commensurate filling.

The dip (peak) in the pairing (CDW) correlation functions observed in the LDA may be understood from the CDW-pairing degeneracy that exists precisely at half-filling, and the corresponding suppression of the finite- $T$  pairing order that exists away from half-filling. While the LDA compares favorably with the *ab initio* calculation across most of the lattice, the dip (peak) in the  $s$ -wave pairing (CDW) when the  $\rho(i) = 1$  ring is crossed is conspicuously absent in the true trapped system.

It is useful to compare this behavior with the RHM, where the physics of commensurate filling ( $\rho = 1$ ) can be inferred correctly, for the most part, from the LDA because of the presence of an annulus of finite thickness which “protects” the Mott region. By contrast, in the AHM, there is no such protection; the half-filled ring is truly one-dimensional, and the physics of commensurate filling is essentially absent in the trap.

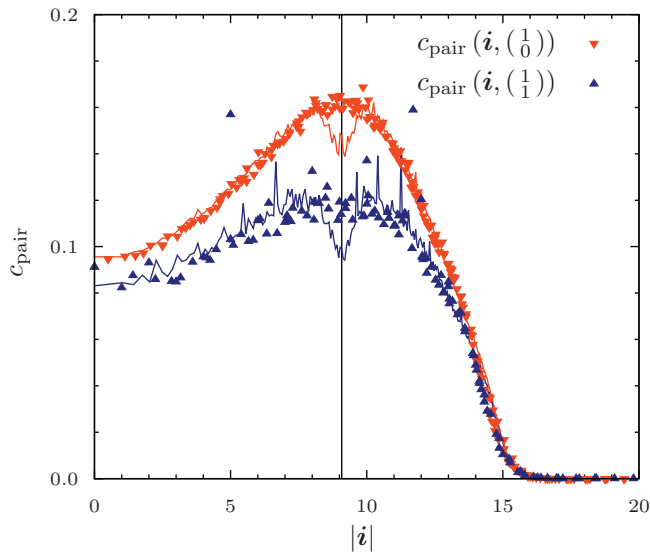


FIG. 2. (Color online) Near-neighbor [ $c_{\text{pair}}(i, (\frac{1}{0}))$ ] and next-neighbor [ $c_{\text{pair}}(i, (\frac{1}{1}))$ ]  $s$ -wave pair correlations as a function of distance  $|i|$  from the trap center, with  $N = 564$  particles,  $U = 6$ ,  $V_{\text{trap}} = 0.0097$ , and  $\mu = 0.8$  at  $\beta = 9$ . The solid lines show the LDA result; in this case, a striking failure of the LDA is seen around half-filling (marked by the vertical line). Due to CDW/ $s$ -wave degeneracy at half-filling in the homogeneous model, the LDA predicts superfluidity only sufficiently far from that point, while in the trapped system the superfluid phase may penetrate the half-filled ring. Error bars have been suppressed to avoid clutter, but the spread of the data points gives an indication of the uncertainties, which result from large statistical fluctuations observed at low  $T$  (see text).

Once again, a deeper understanding can be reached by applying the PH transformation: the  $B = 0$  region of the corresponding RHM divides, and is coupled to, regions where the spins are tilted out of the  $xy$  plane in opposite directions. Spins in the  $B = 0$  region can then lower the system's energy by aligning with neighboring spins on the  $xy$  plane and therefore breaking the local  $SU(2)$  symmetry characteristic of the Hubbard model in the absence of an external field. In the original language of the AHM this implies that, at half-filling, one should expect a reduction of the CDW correlation, an increase in the pairing correlations, and a breaking of the CDW-pairing degeneracy.

For optical-lattice experiments that aim to emulate the Hubbard model, our findings indicate that the physics of the half-filled AHM will be inaccessible in any experimental setup that leads to a confining potential  $(\mu - V_{\text{trap}}|i|^2)$  as in Eq. (1). It has recently been suggested<sup>34</sup> to simulate the AHM on an optical lattice, and then utilize the PH transformation, Eq. (5), to draw conclusions about the repulsive case. However, this proposal appears to be challenging, since the effective absence of the half-filled case in the confined AHM means that the physics of the RHM at zero Zeeman field will be inaccessible.

Both problems outlined above could be solved by the recently suggested “off-diagonal” confinement (ODC),<sup>35</sup> if realized, since particle-hole symmetry indicates that the inhomogeneous lattice can be made uniformly half-filled under ODC. On the other hand, in the conventional “diagonal confinement,” observing a finite-temperature transition to a

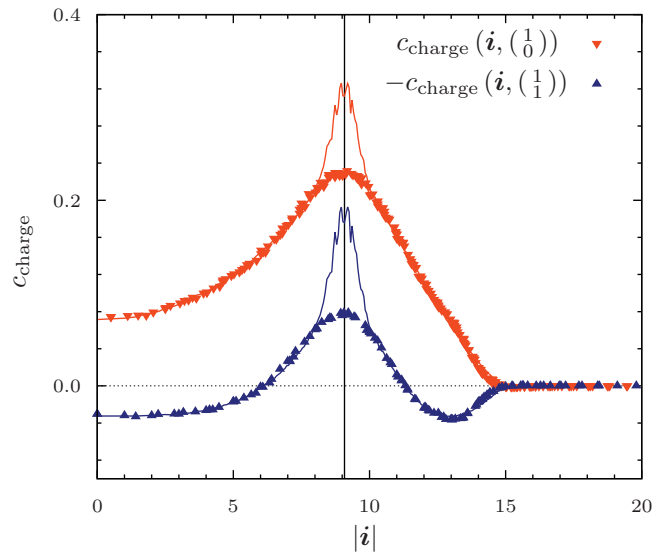


FIG. 3. (Color online) Near neighbor [ $c_{\text{pair}}(i, (\frac{1}{0}))$ ] and next-neighbor [ $c_{\text{pair}}(i, (\frac{1}{1}))$ , with the sign inverted for clarity] CDW correlations as a function of distance  $|i|$  from the trap center, with  $N = 564$  particles,  $U = 6$ ,  $V_{\text{trap}} = 0.0097$ , and  $\mu = 0.8$  at  $\beta = 9$ . The solid lines show the LDA result. As with the pair correlation, the LDA fails around half-filling (marked by the vertical line), where it predicts enhanced CDW correlations. Error bars are smaller than the symbols.

superconducting phase in confined systems becomes much more likely when the CDW region only occupies such a limited spatial region, as discussed in detail in the following section.

#### IV. FINITE-SIZE EXTRAPOLATION

We now turn to the interesting issue of the finite- $T$  phase transition in the confined AHM. In general we may ask, when a trapping potential is added to a model that undergoes, e.g., a KT transition in the homogeneous case, how is the nature of that phase transition altered by the trap? In the case of the classical  $XY$  model, it has been shown<sup>36</sup> that the KT transition of the homogeneous model is preserved in many respects in the trapped case. In this section, we present a finite-size extrapolation (FSE) to address the same question for the AHM.

True phase transitions of course can occur only in the thermodynamic limit of infinite system size. In a translationally invariant system, the correct way to perform this limit is familiar and almost trivial: the global density  $\rho = N/L^2$  is kept constant. In the presence of a trap, the correct generalization is to keep the “characteristic density”  $\tilde{\rho} := N/\ell^2$  constant.<sup>37</sup> Here  $\ell = \sqrt{t/V_{\text{trap}}}$  is the natural length scale in the problem, formed by combining the kinetic energy  $t$  and the trap curvature  $V_{\text{trap}}$ . In the finite-size analysis described below, we have used  $\mu = 0.73$  and kept the total chemical potential at the edge of the lattice constant at  $\mu + [(L+1)/2]^2 V_{\text{trap}} = 3.72$ . This leads to  $\ell \propto L$ <sup>36,38</sup> and therefore  $\tilde{\rho} \propto \rho$ , with  $\tilde{\rho} \simeq 6.5$  and  $\rho \simeq 0.5$ .

Of course, since only finite system sizes are accessible numerically, one must invoke a procedure to infer behavior in the thermodynamic limit from finite lattices. Here, we

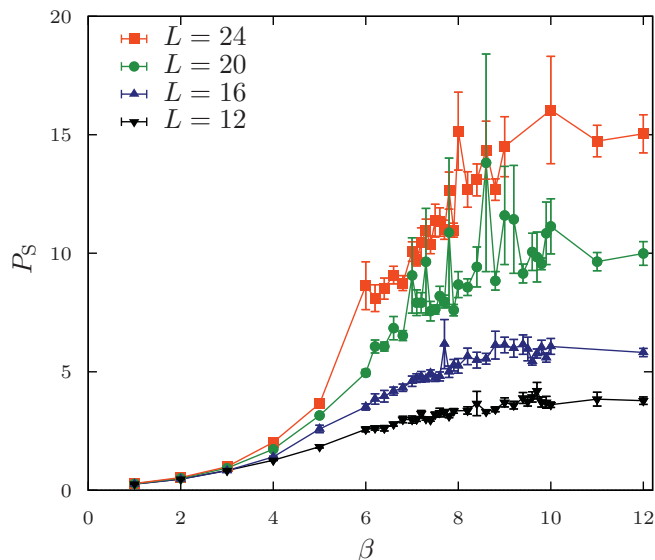


FIG. 4. (Color online) The  $s$ -wave structure factor  $P_S$  for systems of different linear size  $L$  with  $U = 6$  as a function of inverse temperature  $\beta$ . At low temperatures ( $\beta \gtrsim 7$ ), the curves flatten off to values determined by the system size, indicating a divergent correlation length.

follow the finite-size scaling (FSS) procedure discussed in Ref. 33. The generalization of FSS in the presence of the trapping potential has been called *trap-size scaling* (TSS),<sup>38</sup> we note that TSS may be expressed as keeping  $\tilde{\rho}$  constant and proceeding with the FSS analysis as usual.

In this approach, the pair structure factor  $P_S$  of Eq. (3) is obtained for different lattice sizes and temperatures (plotted in Fig. 4). We see that at high temperatures ( $\beta \lesssim 4$ ), when the correlation length is short,  $P_S$  is independent of the system size. At lower temperatures ( $\beta \simeq 4$ ), the curves begin to separate as the correlation length becomes large compared to the system sizes. Finally, for very low temperatures  $P_S$  approaches a constant depending on the system size. This behavior is expected for KT and second-order transitions where observables stop evolving with temperature when the correlation length  $\xi$  exceeds  $L$ .

Unfortunately, the full FSS procedure of Ref. 33 is defeated in the case of the confined AHM because of excessive statistical fluctuations in the DQMC estimator for  $c_{\text{pair}}$ . These large fluctuations are manifest in, for example, the very large error bars in two of the near-neighbor pair correlators of Fig. 2. However, a comparison of results on lattice sizes 12, 14, ..., 24 at temperatures  $1 \leq \beta \leq 16$  provides evidence that the KT transition is indeed preserved in the trap. The approach hinges on the critical scaling of the structure factor in the low-temperature phase; the expected KT form is

$$P_S \sim L^{2-\eta(T)}. \quad (6)$$

The critical exponent  $\eta$  for a KT transition in a homogeneous system is known to vary with temperature between  $\eta(T = 0) = 0$  and  $\eta(T = T_c) = \frac{1}{4}$ .<sup>39</sup> In the trapped system, this issue is complicated by the varying filling. Arguing within the LDA, since the filling varies in the lattice, so does  $T_c$ ; but  $\eta$  must be a function of  $T/T_c$  rather than  $T$  itself, therefore  $\eta$  should vary

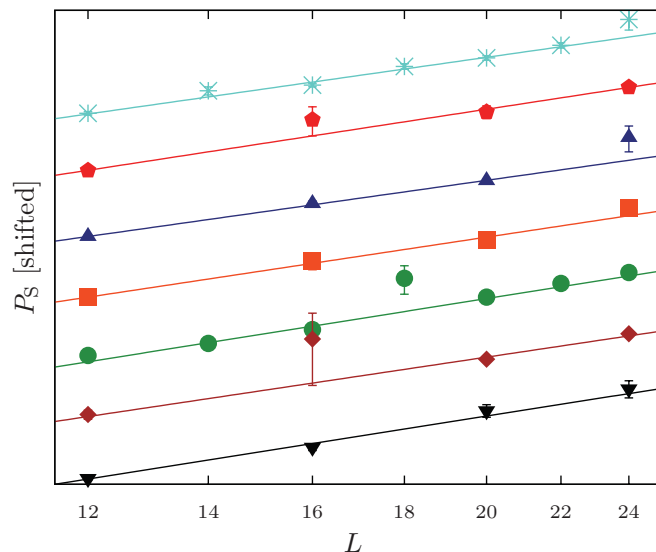


FIG. 5. (Color online) The  $s$ -wave structure factor  $P_S$  as a function of linear lattice size  $L$  for  $U = 6$  at various low temperatures (top to bottom:  $\beta = \frac{1}{7} = 16, 15, \dots, 10$ ) on a doubly logarithmic scale. A vertical shift has been applied to separate the curves from each other. A linear dependence on the doubly logarithmic scale (i.e., the structure factor varies as a power of the system size) is the expected behavior in the low temperature phase of a KT transition.

across the system along with the filling. We must therefore ask whether an effective exponent  $\tilde{\eta}$  exists such that Eq. (6) holds for the system as a whole.

To address this question, we plot  $\log P_S$  as a function of  $\log L$  for several low temperatures,  $\beta \geq 10$ , in Fig. 5. A straight line with slope  $2 - \tilde{\eta}$  in the doubly logarithmic

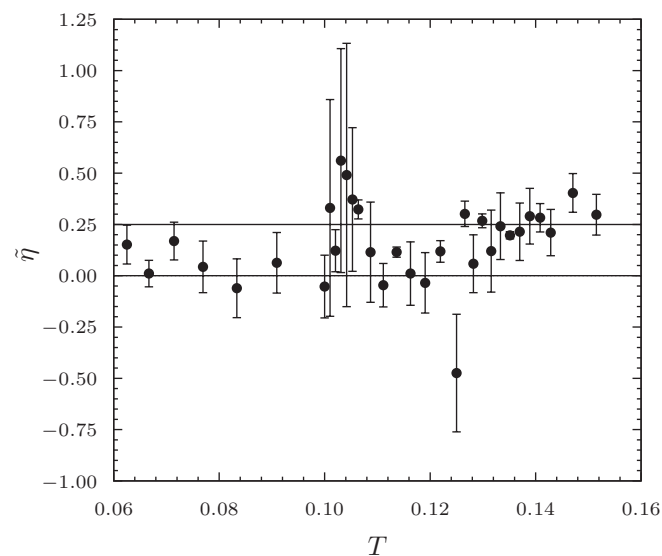


FIG. 6. The effective critical exponent  $\tilde{\eta}$  defined below Eq. (6), as obtained from nonlinear least-squares fits of the data from Fig. 4 to the functional form  $P_S(L; \tilde{\eta}) \propto L^{2-\tilde{\eta}}$ . The horizontal lines indicate the region  $0 \leq \tilde{\eta} \leq \frac{1}{4}$ , expected for the low-temperature phase from the homogeneous case. Although the level of statistical noise is significant across all temperatures  $T$ , the exponent is consistent with values in this range for low temperatures.

plot indicates that the scaling relation, Eq. (6), holds for the whole system with an effective exponent  $\tilde{\eta}$ . Indeed, within the statistical uncertainties, we find good agreement with this expected linear form.

We have used non-linear least-squares fits to estimate  $\tilde{\eta}$  at temperatures  $\beta \geq 6.6$ . Figure 6 shows the results of all fits. Even though there is considerable statistical noise in this plot, relevant features are seen. Most importantly,  $\tilde{\eta}$  is consistent with values in the range  $0 \leq \tilde{\eta} \leq \frac{1}{4}$  in the whole low temperature range depicted in 6, as expected from the KT transition in the homogeneous case. The fitted value of  $\tilde{\eta}$  grows beyond 1/4 at  $T \gtrsim 0.14$ . Around a temperature of  $T \gtrsim 0.1$ , the fluctuations are especially prominent, which may also be interpreted as a signature of the phase transition. Thus, we may estimate the critical temperature of the system as  $T_c \simeq 0.1-0.15$ .

## V. CONCLUSIONS

In this paper, the attractive Hubbard model in a harmonic confining potential was studied, especially with regards to superfluidity at low temperatures. Results from the LDA were compared to calculations within the true trapped system.

While the LDA is valid for local observables in most cases, we find qualitatively wrong predictions for the  $s$ -wave pairing and CDW correlation functions around the ring of half-filling,

where the LDA predicts a dip and a peak, respectively, which are absent when the trapped system is treated *ab initio*. This is linked to the relationship between the pairing and CDW correlations at half-filling, and to the density profile in the trap, where the Mott plateau exhibited by the repulsive Hubbard model is absent. Consequently, the physics of the half-filled case is not represented anywhere in the trap. On the other hand, the suppression of the CDW correlations will make it easier to observe a transition to a superfluid phase at finite temperature.

A finite-size extrapolation, where systems of different sizes but at the same characteristic density  $\tilde{\rho}$  are compared, provides evidence that the Kosterlitz-Thouless transition to a superfluid phase of the homogeneous attractive Hubbard model persists in the trap, with a critical temperature of  $T_c \simeq 0.1-0.15$ .

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<sup>1</sup>P. W. Anderson, *Phys. Rev.* **109**, 1492 (1958).

<sup>2</sup>A. Ghosal, M. Randeria, and N. Trivedi, *Phys. Rev. Lett.* **81**, 3940 (1998); *Phys. Rev. B* **65**, 014501 (2001).

<sup>3</sup>K. Aryanpour, T. Paiva, W. E. Pickett, and R. T. Scalettar, *Phys. Rev. B* **76**, 184521 (2007).

<sup>4</sup>F. Mondaini, T. Paiva, R. R. dos Santos, and R. T. Scalettar, *Phys. Rev. B* **78**, 174519 (2008).

<sup>5</sup>A. F. Hebard, in *Strongly Correlated Electronic Systems*, edited by K. S. Bedell, Z. Wang, D. E. Meltzer, A. V. Balatsky, and E. Abrahams (Addison-Wesley, Reading, MA, 1994), and references cited therein.

<sup>6</sup>B. G. Orr, H. M. Jaeger, A. M. Goldman, and C. G. Kuper, *Phys. Rev. Lett.* **56**, 378 (1986).

<sup>7</sup>R. C. Dynes, J. P. Garno, G. B. Hertel, and T. P. Orlando, *Phys. Rev. Lett.* **53**, 2437 (1984); A. E. White, R. C. Dynes, and J. P. Garno, *Phys. Rev. B* **33**, 3549 (1986).

<sup>8</sup>R. C. Dynes, A. E. White, J. M. Graybeal, and J. P. Garno, *Phys. Rev. Lett.* **57**, 2195 (1986).

<sup>9</sup>M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, *Phys. Rev. B* **40**, 546 (1989).

<sup>10</sup>M.-C. Cha, M. P. A. Fisher, S. M. Girvin, M. Wallin, and A. P. Young, *Phys. Rev. B* **44**, 6883 (1991).

<sup>11</sup>While all optical lattice experiments involve inhomogeneity from the confining potential, in some, randomness, e.g., in the form of laser speckle, is also being deliberately introduced to study the interplay of disorder and interactions.

<sup>12</sup>T. Stöferle, H. Moritz, K. Günter, M. Köhl, and T. Esslinger, *Phys. Rev. Lett.* **96**, 030401 (2006).

<sup>13</sup>J. K. Chin, D. E. Miller, Y. Liu, C. Stan, W. Setiawan, C. Sanner, K. Xu, and W. Ketterle, *Nature (London)* **443**, 961 (2006).

<sup>14</sup>M. Köhl, H. Moritz, T. Stöferle, K. Günter, and T. Esslinger, *Phys. Rev. Lett.* **94**, 080403 (2005).

<sup>15</sup>R. Jördens, N. Strohmaier, K. Günter, H. Moritz, and T. Esslinger, *Nature (London)* **455**, 204 (2008).

<sup>16</sup>U. Schneider, L. Hackermüller, S. Will, T. Best, I. Bloch, T. A. Costi, R. W. Helmes, D. Rasch, and A. Rosch, *Science* **322**, 1520 (2008).

<sup>17</sup>D. J. Scalapino, in *Does the Hubbard Model Have the Right Stuff?*, Proceedings of the International School of Physics, 1992, edited by R. A. Broglia and J. R. Schrieffer (North-Holland, New York, 1994), and references cited therein.

<sup>18</sup>C. N. Varney, C. R. Lee, Z. J. Bai, S. Chiesa, M. Jarrell, and R. T. Scalettar, *Phys. Rev. B* **80**, 075116 (2009); E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, *ibid.* **41**, 9301 (1990).

<sup>19</sup>Y. Fujihara, A. Koga, and N. Kawakami, *J. Phys. Soc. Jpn.* **76**, 034716 (2007).

<sup>20</sup>Y. Chen, Z. D. Wang, F. C. Zhang, and C. S. Ting, e-print [arXiv:cond-mat/0710.5484](https://arxiv.org/abs/cond-mat/0710.5484) (unpublished).

<sup>21</sup>A. Ghosal, M. Randeria, and N. Trivedi, *Phys. Rev. Lett.* **81**, 3940 (1998).

<sup>22</sup>A. Rüegg, S. Pilgram, and M. Sigrist, *Phys. Rev. B* **75**, 195117 (2007).

<sup>23</sup>M. Yamashita and M. W. Jack, *Phys. Rev. A* **76**, 023606 (2007).

<sup>24</sup>A. Koga, T. Higashiyama, K. Inaba, S. Suga, and N. Kawakami, *J. Phys.: Conf. Series* **150**, 032046 (2009).

<sup>25</sup>In solids, the hopping parameter  $t$  can be influenced through the application of pressure.

<sup>26</sup>R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, *Phys. Rev. D* **24**, 2278 (1981).

- <sup>27</sup>H. F. Trotter, *Proc. Am. Math. Soc.* **10**, 545 (1959); M. Suzuki, *Prog. Theor. Phys.* **56**, 1454 (1976); R. M. Fye, *Phys. Rev. B* **33**, 6271 (1986).
- <sup>28</sup>J. E. Hirsch, *Phys. Rev. B* **31**, 4403 (1985).
- <sup>29</sup>E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, *Phys. Rev. B* **41**, 9301 (1990).
- <sup>30</sup>To be precise, the kinetic energy corresponds to  $-t(i)$ . This definition has been chosen to make  $t(i)$  positive.
- <sup>31</sup>J. Ranninger and S. Robaszkiewicz, *Rev. Mod. Phys.* **62**, 113 (1990); R. T. Scalettar, E. Y. Loh Jr., J. E. Gubernatis, A. Moreo, S. R. White, D. J. Scalapino, R. L. Sugar, and E. Dagotto, *Phys. Rev. Lett.* **62**, 1407 (1989); A. Moreo and D. J. Scalapino, *ibid.* **66**, 946 (1991); H. Shiba, *Prog. Theor. Phys.* **48**, 2171 (1972).
- <sup>32</sup>F. F. Assaad, W. Hanke, and D. J. Scalapino, *Phys. Rev. B* **49**, 4327 (1994).
- <sup>33</sup>T. Paiva, R. R. dos Santos, R. T. Scalettar, and P. J. H. Denteneer, *Phys. Rev. B* **69**, 184501 (2004).
- <sup>34</sup>A. F. Ho, M. A. Cazalilla, and T. Giamarchi, *Phys. Rev. A* **79**, 033620 (2009).
- <sup>35</sup>V. G. Rousseau, G. G. Batrouni, D. E. Sheehy, J. Moreno, and M. Jarrell, *Phys. Rev. Lett.* **104**, 167201 (2010). In ODC, the trap is realized as a spatially varying hopping  $t_i$  instead of a spatially varying potential  $\mu_i$ .
- <sup>36</sup>F. Crecchi and E. Vicari, *Phys. Rev. A* **83**, 035602 (2011).
- <sup>37</sup>M. Rigol, A. Muramatsu, G. G. Batrouni, and R. T. Scalettar, *Phys. Rev. Lett.* **91**, 130403 (2003).
- <sup>38</sup>M. Campostrini and E. Vicari, *Phys. Rev. Lett.* **102**, 240601 (2009).
- <sup>39</sup>V. L. Berezinski, *Sov. Phys. JETP* **34**, 610 (1972); J. M. Kosterlitz, *J. Phys. C: Solid State Phys.* **7**, 1046 (1974).