# 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 $V_{\rm trap}$ which makes the density 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 $\rho_{\bf i}$ passes through one fermion per site. In this ring of $\rho_{\bf i} = 1$, charge order is enhanced. A comparison is made between treating $V_{\rm trap}$ 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 determined.

### Introduction

Studies of the interplay of spatial inhomogeneity and superconductivity have a long history. A seminal early result was Anderson's realization[1] 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 Bogliubov-de Gennes approximation,[2,3] Quantum Monte Carlo (QMC)[4,5], and other approaches have quantified the magnitude of disorder which superconductivity can withstand. In these studies, and the granular superconducting materials they model[6] 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 of bosons exist,[7] or breaking of the Cooper pairs themselves.[8] Which mechanism dominates determines the appropriate modeling, e.g. a description within the disordered boson[9] or fermion Hubbard Hamiltonians, or 'phase-only' descriptions with the XY model and its variants.[10]

Recently, experiments on ultra-cold atoms have provided a rather different realization of inhomogeneity in the form of a smoothly varying confining potential which produces a system with maximal density at the trap center, falling to zero at the periphery.[11] Much attention has focussed on repulsively interacting bosons and fermions[40,41]. In this case, a Mott insulator may coexist with superfluid or normal phases. For fermions, the Mott insulator also exhibits antiferromagnetic correlations. At present, experimentally accessible temperatures for fermionic systems are such that a degenerate Fermi gas has been observed[12], along with signatures of the Mott phase.[13,14] The ultimate objective is insight into the ground state physics of the repulsive Hubbard model, and, in particular, the fundamental issue of $d$-wave superconducting order and its interplay with antiferromagnetism.[52]

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. As discussed above, this case is not only of interest its own right, but also QMC simulations can often attain lower temperatures for attractive models, and thus can track experiments closer, and perhaps even down to, transitions into ordered phases.

A central issue in studies of attractive fermions has been the question of superconductivity in systems where the populations of the two species are unequal[15,16] and the nature of the paired phase as originally discussed by Fulde and Ferrell,[17] Larkin and Ovchinnikov[18] and Sarma.[19] Theoretical[20–32] and numerical investigations[33–38] have looked primarily at population imbalance, neglecting the effect of confinement.

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, namely the coexistence of phases as the density varies across the trap.[39] However, the attractive case has several important distinctions, namely the possibility of 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 $\rho = 1$. 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 much smaller spatially, 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, and the LDA 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 for the physics within the Local Density Approximation (LDA), in which the local behavior within a confining potential is assumed to be that of a homogeneous system with global density matching the local filling. Direct simulations of a confined systems are next reported, and compared to those expected from the LDA. 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,[44] Bogliubov de-Gennes,[45]and Gutzwiller approaches.[46,47] Of particular relevance here is work within dynamical mean field theory (DMFT) and a two-site impurity solver[43], which suggested that this degeneracy is stabilized by a confining potential, and that an extended supersolid phase of commensurate density, with simultaneous non-zero CDW and pairing order parameters, exists in a trap.

### Models and Computational Approach

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

$$\hat{H} = -t \sum_{\langle \mathbf{ij} \rangle} (c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}) - |U| \sum_{\mathbf{i}} (n_{\mathbf{i}\uparrow} - \frac{1}{2})(n_{\mathbf{i}\downarrow} - \frac{1}{2}) + \sum_{\mathbf{i}} V_{\rm trap}\big((i_x^2 + i_y^2) - \mu\big)(n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow}) \; . \quad (1)$$

Here $c^{\dagger}_{\mathbf{i}\sigma}(c_{\mathbf{i}\sigma})$ are creation(destruction) operators at spatial site $\mathbf{i}$ for two different species of fermions $\sigma$. We choose the center of the trap to be at a plaquette center, so that $i_x, i_y$ 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, or, in solids, through the application of pressure. $\langle \mathbf{ij} \rangle$ is a sum over near neighbor pairs of sites. Here $t = 1$ is chosen to set the scale of energy. $|U|$ is the on-site attraction, and can be tuned through the application of a magnetic field via a Feshbach resonance. In Eq. 1, $V_{\rm trap}$ and $\mu$ are the trap curvature and chemical potential respectively. The latter can be used to get a desired particle number $N_{\rm fermion}$.

In DQMC[48,49] the partition function $Z = {\rm Tr}\, e^{-\beta \hat{H}}$ is written as a path integral by discretizing the inverse temperature $\beta$ into $L_\tau$ intervals of size $\Delta\tau = \beta/L_\tau$. The Trotter approximation $e^{-\Delta\tau \hat{H}} \approx e^{-\Delta\tau \hat{K}} e^{-\Delta\tau \hat{V}}$ isolates the quartic terms (involving the interaction $U$) in $\hat{H}$, and a discrete Hubbard-Stratonovich field[50] 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 of dimension the number of lattice sites, $L^2$. Because the two species couple to the Hubbard-Stratonovich field with the same sign in the case of attractive $U$, the two determinants are identical and there is no sign problem.This allows us to study confined systems down to arbitrarily low temperatures, unlike the repulsive model where the largest $\beta$ accessible is $\beta \approx 3-4$ for $t = 1$ and $U = 4-8$ for confined systems.[39]

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

$$\begin{aligned} c_{\rm pair}(\mathbf{i},\mathbf{j}) &= \langle \Delta_{\mathbf{i}+\mathbf{j}} \Delta^{\dagger}_{\mathbf{i}} \rangle \qquad \Delta^{\dagger}_{\mathbf{i}} = c^{\dagger}_{\mathbf{i}\uparrow} c^{\dagger}_{\mathbf{i}\downarrow} \\ c_{\rm charge}(\mathbf{i},\mathbf{j}) &= \langle n_{\mathbf{i}+\mathbf{j}} n_{\mathbf{i}} \rangle - \langle n_{\mathbf{i}+\mathbf{j}} \rangle \langle n_{\mathbf{i}} \rangle \qquad n_{\mathbf{i}} = n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow} \end{aligned} \quad (2)$$

Notice that these depend on $\mathbf{i}$ and not just on the separation $\mathbf{j}$. We also define the associated ('local') structure factors,

$$\begin{aligned} P_{\rm s}(\mathbf{i}) &= \sum_{\mathbf{j}} c_{\rm pair}(\mathbf{j}) \\ S_{\rm cdw}(\mathbf{i}) &= \sum_{\mathbf{j}} (-1)^{\mathbf{j}}\, c_{\rm charge}(\mathbf{j}) \end{aligned} \quad (3)$$

It is useful to review the properties of the translationally invariant case, $V_{\rm trap} = 0$. In two dimensions, it is known that the half-filled attractive Hubbard Hamiltonian has long range CDW and $s$-wave pairing order in its ground state $T = 0$.When doped, the symmetry between charge and pairing is broken, and a finite temperature (Kosterlitz-Thouless) transition occurs to a superconducting phase. Numerical and analytic studies show that $T_c$ rises rapidly as $\mu$ is made non-zero and reaches a maximum value of $T_c \approx t/10$ for a wide range of fillings $0.5 \lesssim \rho \lesssim 0.9$.

Consideration of a particle-hole (PH) transformation helps clarify these assertions. When the down spin operations in the AHM, Eq. 1 are mapped with $c_{\mathbf{i}\sigma} \leftrightarrow (-1)^{\mathbf{i}} c^{\dagger}_{\mathbf{i}\sigma}$, the kinetic energy is unchanged, as long as the lattice is bipartite. The phase factor $(-1)^{\mathbf{i}}$ is understood to take the values $+1(-1)$ on the $A(B)$ sublattices. The interaction term changes sign, so that the AHM maps onto the RHM. This PH symmetry provides a simple argument that the half-filled AHM can have long range order (LRO) only at $T = 0$ in two dimensions, like the RHM.

QMC simulations have shown that the ground state of the half-filled, two-dimensional uniform RHM is ordered.[50] 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 $n_{\mathbf{i}\uparrow} - n_{\mathbf{i}\downarrow}$ in the RHM maps onto the charge $n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow}$ 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 transformation is the explanation of the occurrence of pairing order (and the absence of CDW order) at finite $T$ in the doped AHM. When doped, $\mu$ is non-zero. Under the PH transformation, the chemical potential term $\mu(n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow})$ in the AHM becomes a Zeeman field $\mu(n_{\mathbf{i}\uparrow} - n_{\mathbf{i}\downarrow})$ in the RHM. Because the magnetic 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 means $s$-wave pair order occurs in the AHM.

### Correlations in Confined Fermi Systems and the Local Density Approximation

The following text will be modified as we decide which way best to present the figures.

We begin by showing the density profile in Fig. 1. Results are given both in the LDA and in a trapped $30 \times 30$ system with $\mu = 0.8$ and $V_{\rm trap} = 0.0097$. These two approaches yield results in very good agreement for $\rho_{\mathbf{i}}$. An important point is the absence of a density plateau at $\rho = 1$. This is 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. Fig. 1 shows the density as a function of chemical potential for homogeneous systems.

As noted above, the AHM has finite compressibility at integer filling. There is no Mott plateau at half-filling. This true one-dimensionality of the $\rho = 1$ 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-2d integer filling Mott annulus that occurs in the RHM. On the other hand, that the CDW region occupies such a limited spatial region makes the possibility of observing a finite-temperature transition to a superconducting phase in confined systems much more likely. Indeed, Fig. 2 illustrates the suppression of pairing which according to the LDA (solid line). Near-neighbor $c_{\rm charge}(\mathbf{i}, (1,0)$ ) and next-near neighbor $c_{\rm pair}(\mathbf{i}, (1,1))$ dip at $r/d = 1$, where the local density $\rho_{\mathbf{i}} = 1$, as do the farthest neighbor correlators and the local structure factor $P_{\rm s}(\mathbf{i})$. Fig. 3 shows the density correlators $c_{\rm charge}(\mathbf{i}, (1,0))$ and $c_{\rm charge}(\mathbf{i}, (1,1))$ which peak as the system crosses through commensurate filling.

In Figs. 2 and 3, we also show the values for the s-wave pair and CDW correlation functions in the presence of a real trap, ie. not within the LDA, for a $30 \times 30$ system with $\mu = 0.8$ and $V_{\rm trap} = 0.0097$. While they are rather similar to the LDA results (solid lines), the dip in the s-wave pairing when the $\rho_{\mathbf{i}} = 1$ ring is crossed is conspicuously absent. This is one of the key results of this paper, and may be understood as follows: In the RHM, 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. In the AHM, in contrast, there is no such protection. The ring of commensurate filling is truly one-dimensional, and therefore irrevocably coupled to doped regions. Apparently, the dips in the pairing which are so evident in the LDA treatment simply cannot survive this linkage.

### System-Size Dependence of Correlations and Quasi-Long-Range Order

In a translationally invariant system, lattices of different linear size $L$ are compared at fixed density $\rho = N_{\rm fermion}/L^2$. In the presence of a trap, systems with different particle number can be compared if the "characteristic density" $\rho_c = N_{\rm fermion}/L_c^2$ is kept constant.Here $L_c = \sqrt{V_{\rm trap}/t}$ is the natural length scale in the problem, formed by combining the kinetic energy $t$ and the trap curvature $V_{\rm trap}$. For the comparison of different system sizes described below, we

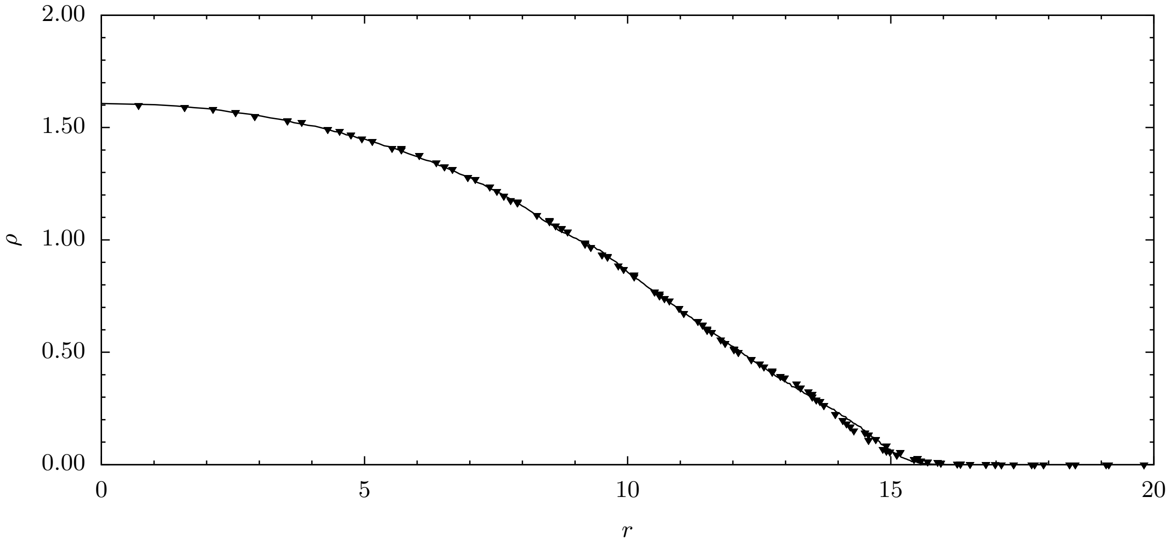


FIG. 1: Fermion density versus radius in a trapped $30 \times 30$ system with $V_{\rm trap} = 0.0097$ at $|U| = 6$, $\beta = 9$. The solid line is the LDA result.

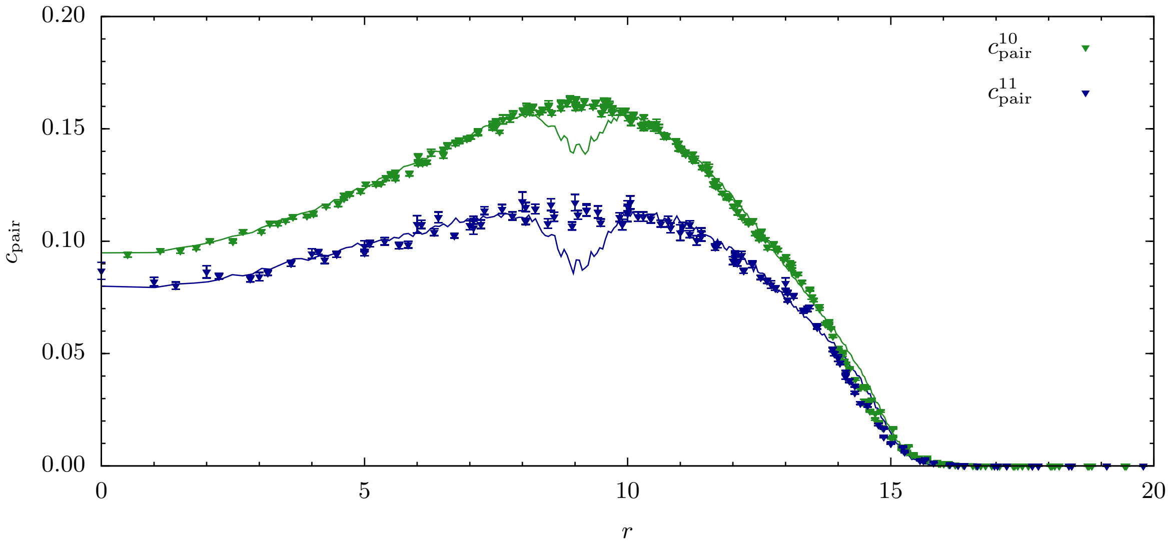


FIG. 2: S-wave pair correlation function versus radius in a trapped $30 \times 30$ system with $V_{\rm trap} = 0.0097$ at $|U| = 6$, $\beta = 9$. The solid line is the LDA result.

have used systems of constant $\rho_c$. Note that this can be achieved by keeping the chemical potential at the edge of the system, $\mu - V_{\rm trap}(L/2)^2$, constant.

We now turn to the interesting question of ordering at low temperatures in these confined gases. As noted before, the homogeneous AHM undergoes a Kosterlitz-Thouless transition to a quasi-long-range-ordered phase at finite $T_{\rm c}$. For a detailed finite size scaling of the homogeneous model is presented in [53]. In this approach, the pair structure factor $P_{\rm s}$ of Eq. 3 is obtained for different lattice sizes and temperatures (at fixed $\rho_c$). The scaled structure factor $L^{-7/4}P_{\rm s}$ is then plotted as a function of the ratio of lattice size to correlation length, $L/\xi = L\,\exp(-A/(T-T_{\rm c})$ with the expected Kosterlitz-Thouless form for the temperature dependence of $\xi$, and also the fact that the structure factor is expected to grow with lattice size as

$$P_S \sim L^{2-\eta(T)} f(L/\xi) \tag{4}$$

with a scaling function $f$ and the critical exponent $\eta$ varying between $\eta(0) = 0$ at zero temperature and $\eta(T_{\rm c}) = 1/4$ at the transition temperature.

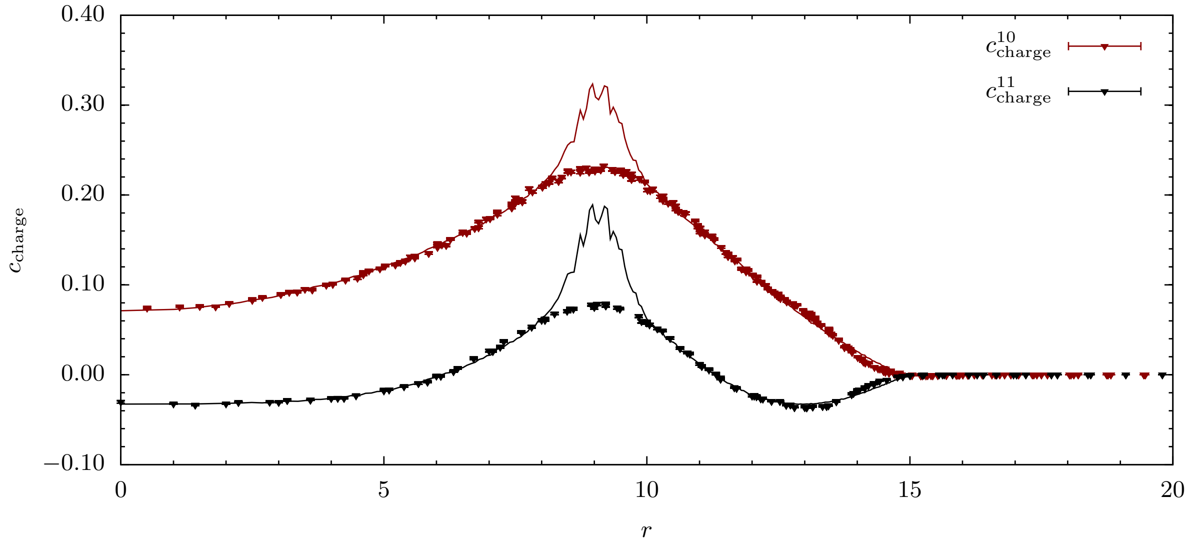


FIG. 3: CDW correlation function versus radius in a trapped $30 \times 30$ system with $V_{\rm trap} = 0.0097$ at $|U| = 6$, $\beta = 9$. The solid line is the LDA result.

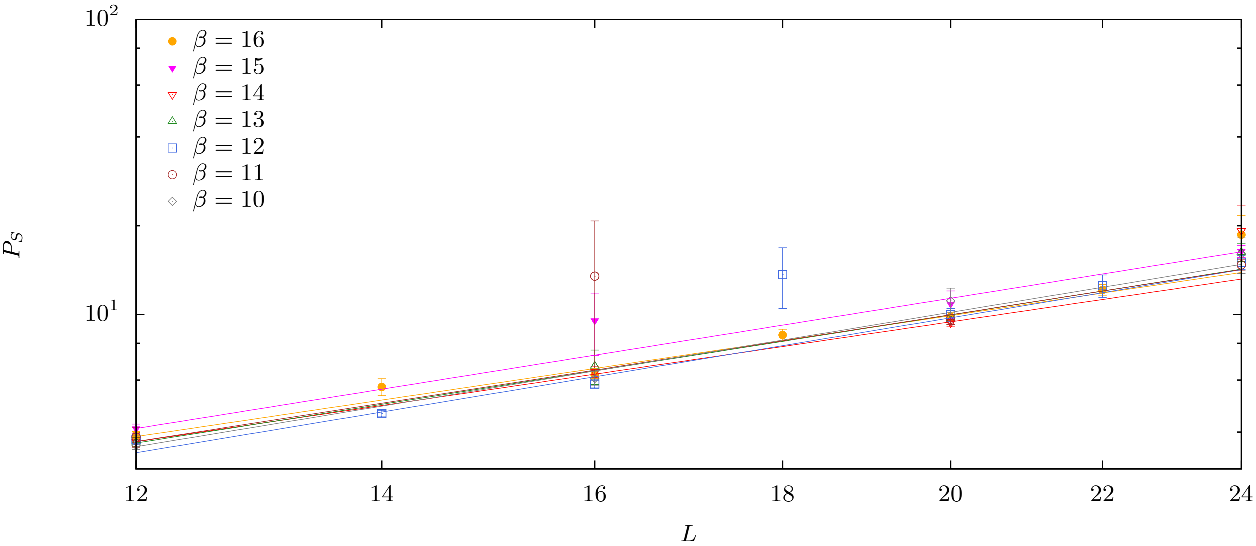


FIG. 4: Pair structure factor as a function of linear system size for $\beta = 10, 11, \ldots 16$ with fits of the form of the scaling relation (4).

A complete finite-size scaling for the trapped AHM is beyond the scope of this paper. Because of the temperature dependence of the critical exponent $\eta$, it is unclear whether the scaling relation (4) holds in this case. In the framework of the LDA, the spatial variation of the density and the dependence of $T_{\rm c}$ on the density would lead to a variation of $\eta$ along the radius in the trap. Only if an "effective $\eta$" exists, for which (4) holds, can the finite-size scaling be carried out in close analogy to the homogeneous case. We show in Fig. 4 the structure factor as a function of linear system size for various low temperatures. If the scaling relation holds, we expect straight lines on the double-logarithmic plot for low temperatures. Fig. 4 indeed suggests that (4) holds with $\eta \approx 0.05 \pm 0.15$.

Finally, Fig. 5 shows the structure factor for various system sizes as a function of inverse temperature. At low temperatures, systems of all size behave similarly, suggesting only short-range order exists; at $\beta \gtrsim 10$, $P_S$ saturates to values depending on the system size, suggesting a diverging correlation length $\xi$ and quasi-long-range order.

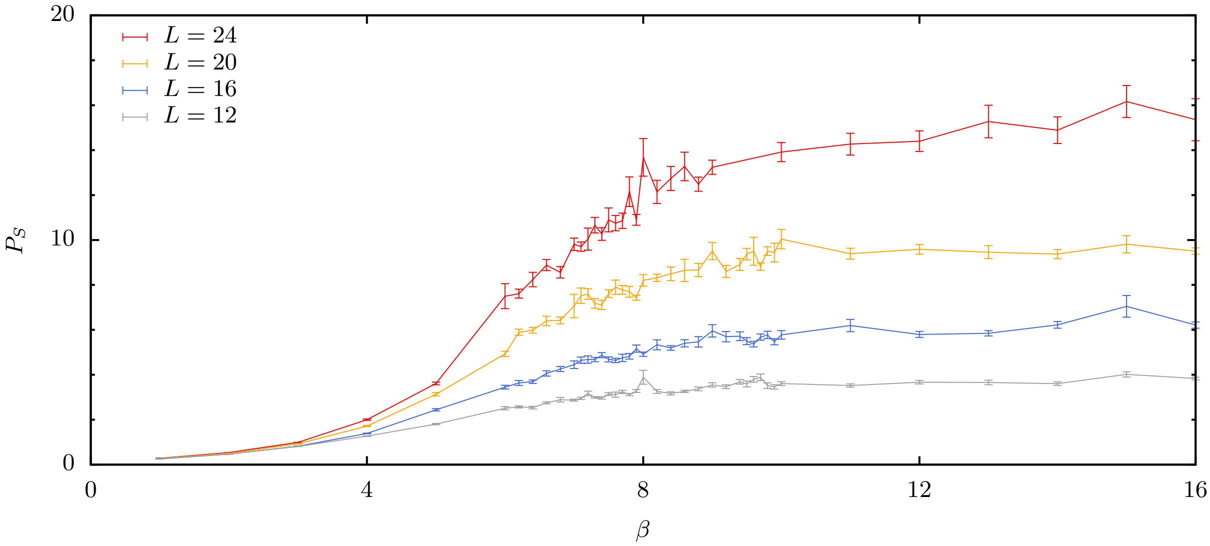


FIG. 5: Pair structure factor as a function of inverse temperature for various system sizes.

## Conclusions

We have shown that the Local Density Approximation for the trapped attractive Hubbard model fails in the case of s-wave pairing and charge-density-wave correlation functions around half-filling. This failure is due to the degeneracy of s-wave pairing and charge-density-wave ordering at half-filling, and the fact that the half-filled ring in this model is truly one-dimensional.

By a comparison of trapped systems of different sizes (at constant characteristic density), we have argued that the quasi-long-range-ordered phase of the homogeneous model is preserved in the trapped case.

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