# Optimized confinement of fermions in two dimensions

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(Received 16 December 2011; revised manuscript received 27 January 2012; published 21 February 2012)

One of the challenging features of studying model Hamiltonians with cold atoms in optical lattices is the presence of spatial inhomogeneities induced by the confining potential, which results in the coexistence of different phases. This paper presents quantum Monte Carlo results comparing methods for confining fermions in two dimensions, including conventional diagonal confinement, a recently proposed "off-diagonal confinement", as well as a trap which produces uniform density in the lattice. At constant entropy and for currently accessible temperatures, we show that (1) diagonal confinement results in the strongest signature of magnetic order, primarily because of its judicious use of entropy sinks at the trap edge and that (2) for d-wave pairing, a trap with uniform density is optimal and can be effectively implemented via off-diagonal confinement. This feature is important to any prospective search for superconductivity in optical lattices.

DOI: 10.1103/PhysRevB.85.075418 PACS number(s): 67.85.−d, 05.30.Fk, 71.10.Fd, 71.27.+a

## I. INTRODUCTION

Optical lattice emulators (OLE) control ultracold atomic gases with lasers and magnetic fields to create experimental realizations of quantum lattice models of bosonic or fermionic particles. For bosons, classic signatures of low temperature correlated states—superfluidity and the Mott transition—have been explored now for a decade.[1] For fermions, quantum degeneracy has been established through the observation of a Fermi surface,[2] as has the Mott transition.[3,4] The observation of magnetic order is the next immediate experimental objective.[5–8] One ultimate goal is resolving the long-standing question of whether the doped two-dimensional (2D) fermion Hubbard Hamiltonian has long-range $d$-wave superconducting order.[9]

Optical lattice experiments face at least two major obstacles in simulating the fermion Hubbard model. The first is achieving low enough temperature to pass through phase transitions and into reduced entropy ordered phases. Present limits in experiments are to temperatures $T \sim t$ (the near-neighbor hopping energy), and to local entropies per atom $\sim 0.77 k_B$,[10] values which are at the border for observing short-range magnetic order.

The other obstacle, which we will be addressing in this paper, is inhomogeneity arising from the confining potential.[11] The external field conventionally used to trap cold atoms in the lattice, a spatially dependent chemical potential which we refer to as "diagonal confinement" (DC), causes variations in the density per site $\rho_{\mathbf{i}}$, with more atoms, on average, in the center of the lattice and fewer at the edges. Density plays a key role in determining which correlations are dominant in interacting quantum systems, but this is especially true of the fermion Hubbard Hamiltonian in two dimensions where the magnetic response is very sharply peaked[12] near half-filling ($\rho = 1$). Various analytic and numerical calculations suggest that pairing order also has a fairly sharp optimal filling, $\rho \approx 0.80 - 0.85$.

As a consequence of the inhomogeneous density arising from DC, a trapped gas in an optical lattice will exhibit coexistence of different phases, complicating the analysis and, potentially, significantly weakening and blurring the signal of any phase transitions. To some extent, this loss of signal is reduced for antiferromagnetism (AFM), since the Mott gap in a DC trap can produce a fairly broad region of half-filling, where AFM is dominant. But the problem of observing pairing order with DC seems especially acute since there is no such protection of the optimal density for superconductivity.

A recent proposal[13] to use a reduction to zero of the hopping at the lattice edge to confine the atoms allows the realization of systems with more uniform density. Such control of hopping parameters is experimentally possible through holographic masks[14] and is referred to as "off diagonal confinement" (ODC). Since ODC preserves the particle-hole symmetry of the unconfined Hubbard Hamiltonian, this trapping geometry can lead to a uniform $\rho = 1$ density and, at low entropy, can produce a pure antiferromagnetic phase.

What is unclear is whether ODC is an effectively superior way to confine fermions in OLE. This is a nontrivial question since OLE experiments do not have direct control over the temperature—instead, the lattice and trapping potentials are introduced adibatically, so optical confinement methods must be compared at fixed entropy. Here we present determinant quantum Monte Carlo (DQMC)[15] calculations which compare systems with ODC and DC traps, as well as a proposed melding of these confinement methods to create a constant density (CD) trap. We evaluate the effects of these traps on magnetic order and $d$-wave pairing correlations across the lattice.

Our key results are (1) that the conventional DC trap yields larger spin correlations than an ODC trap at the same, currently accessible entropy, (2) that, however, under the same conditions, a constant density trap leads to larger pairing correlations than those achievable with DC traps, and (3) that ODC can implement a near constant density profile.

 

## II. TRAPPED HUBBARD MODEL, COMPUTATIONAL METHODS

The Hubbard Hamiltonian in the presence of spatially varying hopping and chemical potential is

$$H = -\sum_{\langle \mathbf{ij}\rangle,\sigma} t_{\mathbf{ij}}\,(c^\dagger_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma} + c^\dagger_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma}) + U\sum_{\mathbf{i}}\left(n_{\mathbf{i}\uparrow}-\frac{1}{2}\right)\left(n_{\mathbf{i}\downarrow}-\frac{1}{2}\right) - \sum_{\mathbf{i}}\mu_{\mathbf{i}}\,(n_{\mathbf{i}\uparrow}+n_{\mathbf{i}\downarrow}). \quad (1)$$

Here $c^\dagger_{\mathbf{i}\sigma}$ ($c_{\mathbf{i}\sigma}$) are creation (destruction) operators for two fermionic species $\sigma$ on site $\mathbf{i}$, and $n_{\mathbf{i}\sigma}$ are the corresponding number operators. We will study a two-dimensional (2D) square lattice with hopping between pairs of near neighbor sites $\langle \mathbf{ij}\rangle$. For a DC trap, $t_{\mathbf{ij}}$ is constant and the chemical potential $\mu_{\mathbf{i}} = \mu_0 - V_t(i_x^2 + i_y^2)$ decreases quadratically toward the lattice edge. For an ODC trap, instead, $\mu_{\mathbf{i}}$ is constant and the hopping term varies. Here we choose a parabolic form $t_{\mathbf{ij}} = t_0 - \alpha\, r^2_{\text{bond}}$, where $r_{\text{bond}}$ is the distance of the center of bond $\langle \mathbf{ij}\rangle$ to the lattice center.[13] Particle-hole symmetry for this geometry implies the density $\rho_{\mathbf{i}} = \langle \sum_\sigma c^\dagger_{\mathbf{i}\sigma}c_{\mathbf{i}\sigma}\rangle = 1$ for all lattice sites when $\mu_{\mathbf{i}} = 0$.

For ODC, we fix energy units by setting $t_0 = 1$ at the lattice center. The parameter $\alpha$, which controls the hopping decay, is chosen so that $t_{\mathbf{ij}} \to 0$ at the edge. A similar convention is used for the CD trap, with the addition that now $V_t$, as well as $\alpha$, is nonzero.

We characterize and compare traps using the nearest-neighbor (n.n.) spin-spin correlation, $m$, and the next-nearest-neighbor (n.n.n.) $d$-wave pairing correlation, $p$. These are defined as:

$$S^+_{\mathbf{i}} = c^\dagger_{\mathbf{i}\uparrow}c_{\mathbf{i}\downarrow} \quad \Delta^\dagger_{\mathbf{i}} = c^\dagger_{\mathbf{i}\uparrow}(c^\dagger_{\mathbf{i}+\hat{x}\downarrow} - c^\dagger_{\mathbf{i}+\hat{y}\downarrow} + c^\dagger_{\mathbf{i}-\hat{x}\downarrow} - c^\dagger_{\mathbf{i}-\hat{y}\downarrow})$$
$$m(\mathbf{i}) = \langle S^-_{\mathbf{i}+\hat{x}}S^+_{\mathbf{i}}\rangle \quad p(\mathbf{i}) = \langle \Delta_{\mathbf{i}+\hat{x}+\hat{y}}\Delta^\dagger_{\mathbf{i}}\rangle. \quad (2)$$

## III. USE OF LDA TO SIMULATE TRAPS

To simulate different traps, we first compute observables and entropy values for homogeneous $8\times 8$ lattices using DQMC[15] which provides exact results for operator expectation values of the fermion Hubbard Hamiltonian.[16] The entropy is obtained via energy integration from $T = \infty$ and values obtained are consistent with other recently published results.[17,18]

We then use the local density approximation to simulate the effects of each trapping method for a much larger lattice. With the LDA, observables for any position in a trap are determined by the density ($\rho$) of the equivalent homogeneous system, that is, a system with the same values for $U/t$, $mu/t$, and $T/t$ as the local point in the trapped lattice. So, for each trap, we compute these values at each position (as a function of $r$) and determine the spin and $d$-wave pairing correlation, $m(r)$ and $p(r)$, from the equivalent homogeneous result. The accuracy of the LDA for short-range correlation functions has been demonstrated for 2D[19] and 3D[20,21] lattices in the regime of temperature presently considered.

For a trap at a given temperature, the number of fermions ($N$) and total entropy ($S$) are obtained by integrating the site density $\rho(r)$ or entropy per site $s(r)$ across the lattice: $N = 2\pi\int_0^\infty r\rho(r)\,dr$ and $S = 2\pi\int_0^\infty rs(r)\,dr$. Discrete lattice sums are not used, since the simulated lattice sizes (approximately 11 000 sites for $r = 60$) are large enough that the functions $\rho(r)$ and $s(r)$ can be considered continuous.

## IV. COMPARING DIFFERENT TYPES OF TRAPS

Figures 1 and 2(a) show the variation of the density ($\rho$) and entropy per site with $U/t$ and $\mu/t$ for the uniform Hubbard model at $T/t = 0.5$. Different trapping geometries correspond to the different paths in the ($\mu$,$U$) plane. Figures 2(b) and 2(c) show, respectively, the variations in n.n. spin and n.n.n. $d$-wave correlations for the 2D Hubbard model. The arrows in Figs. 2(b) and 2(c) indicate the trajectories of sample trap paths projected onto the $U/t - \mu/t$ plane. Note that these figures are at a specific temperature ($T/t = 0.5$), while for an actual trap path (ODC, for example), $T/t$ will vary across the lattice; in what follows, we compare traps with the same entropy, *not* at the same temperature.

The four parameters $U/t_0$, $\mu_0/t_0$, $V_t/t_0$, and $\alpha/t_0$ determine the shape and physics for each trap type with the following constraints: DC, $\alpha = 0$; ODC, $V_t = 0$; and CD, $V_t$ and $\alpha$ chosen to approximately follow a constant density path. To estimate the pairing and magnetic order for a certain confinement type, we use the average, per particle, of the quantities in Figs. 2(b) and 2(c): the average n.n.n. d-wave pairing correlation for superfluidity $\langle p\rangle = \frac{2\pi}{N}\int_0^\infty rp(r)\,dr$, and the average n.n. spin correlation for magnetism $\langle m\rangle = \frac{2\pi}{N}\int_0^\infty rm(r)\,dr$.

We first determined the optimal $U$, $\mu_0$, $V_t$, and $\alpha$ for each trap type (DC, ODC, CD) by selecting the parameter values yielding traps that maximize either $\langle p\rangle$ or $\langle m\rangle$. Once the optimal parameters were identified by trap type, we proceed to

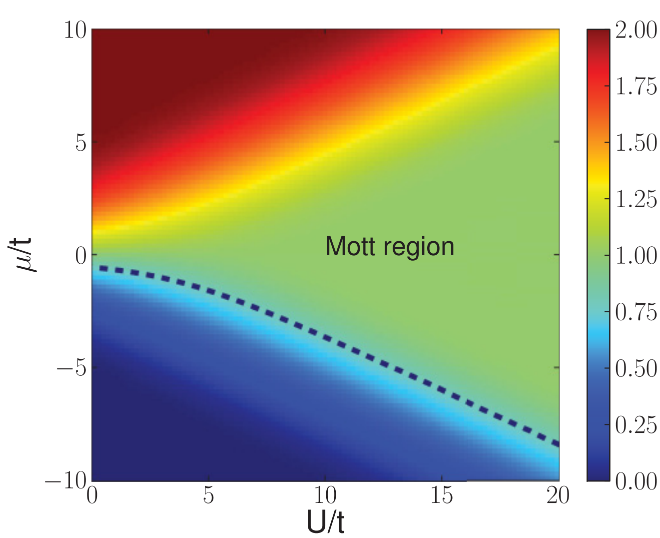


FIG. 1. (Color online) The density as a function of $U/t$ and $\mu/t$ for the homogeneous fermion Hubbard model. Data were obtained on $8\times 8$ lattices with $T/t = 0.5$. The dotted line is a constant density path ($\rho = .80$) used in the trap comparisons. Using the LDA, density profiles of inhomogeneous models can be determined by following an appropriate ($U/t$,$\mu/t$) path of local parameters as the lattice position is changed.

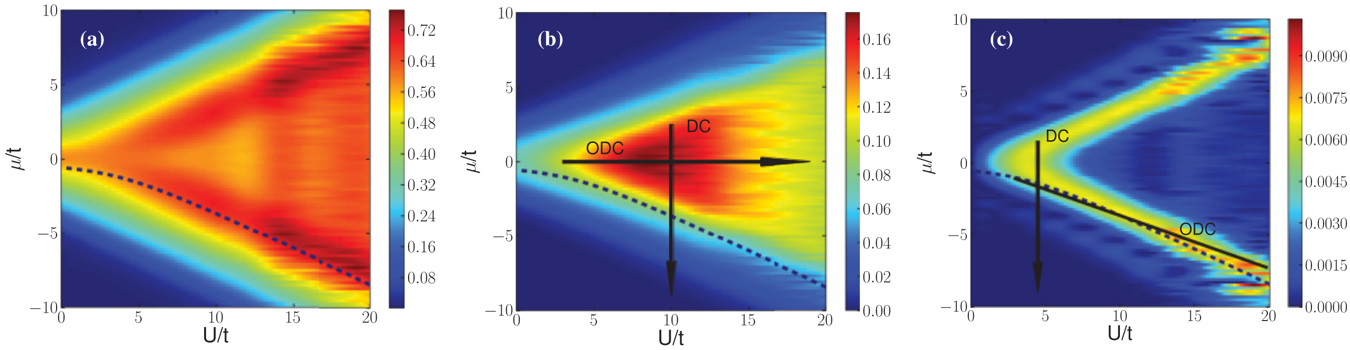


FIG. 2. (Color online) (a) Entropy per site, (b) n.n. spin correlation, and (c) n.n.n. $d$-wave pairing correlation shown as functions of $U/t$ and $\mu/t$ for the homogeneous Hubbard Hamiltonian. Data were obtained on $8 \times 8$ lattices with $T/t = 0.5$. Paths for optimal DC and ODC traps are shown as solid lines, with the constant density trap (CD) as a dashed line. The ridge of prominent $d$-wave pairing (c) occurs at $\rho \sim 0.80$ and is nearly linear, so that an ODC path is close to the constant density one.

compare traps of different types. In all comparisons, the total number of fermions and total entropy are the same for each trap.

## V. MAGNETIC ORDER

Figure 3 compares an optimal DC trap ($U = 10.0, \mu_0 = 2.5, V_t = 0.0039$) with an optimal ODC trap ($U = 3.0, \mu_0 = 0.0, \alpha = 0.0004$). Both parameter sets were selected by maximizing $\langle m \rangle$ under the common constraints $S/N = 0.75$ and $N = 6600$. Note that the figure panels show only two trap types since, when $\mu_0 = 0.0$, the ODC trap is equivalent to the $\rho = 1$ CD trap.

One might expect ODC to lead to large antiferromagnetic correlations, since this confinement method allows for a uniform half-filled Mott phase where magnetic correlations are strongest. However, as Fig. 3(a) shows, DC has a significantly larger average spin correlation (0.14 vs 0.08) than ODC when the two are compared at the same entropy.

This results because the low density wings in the DC trap can store entropy that would otherwise accumulate in region nearer the trap center. The central area in the DC trap is effectively at lower temperature and has higher spin correlations than in an ODC trap where there is no entropy sink in the wings. Consequences of nonuniform entropy distribution have been emphasized previously in Refs. 17 and 18.

## VI. PAIRING AWAY FROM HALF-FILLING

We now turn to the question of pairing order. In Fig. 4, we show results comparing average next-near-neighbor[22] $d$-wave pairing correlation for optimal DC, ODC, and constant density

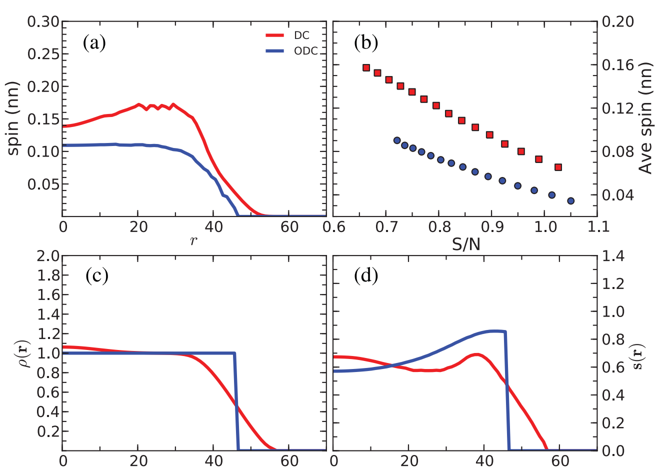


FIG. 3. (Color online) (a) n.n. spin correlation, (c) density ($\rho$), and (d) entropy per site ($s$) profiles are shown as a function of the distance ($r$) from the trap center for two different trap types: DC and ODC, using optimal trap parameters. ODC trap with $\mu = 0.0$ is also a constant density trap ($\rho = 1$). The average n.n. spin correlation is larger for DC trap (0.14) than ODC (0.08) at the same entropy (0.75) and number of fermions (6600). Panel (b) shows average n.n. spin correlation as a function of entropy per fermion ($S/N$) for optimal DC and ODC traps.

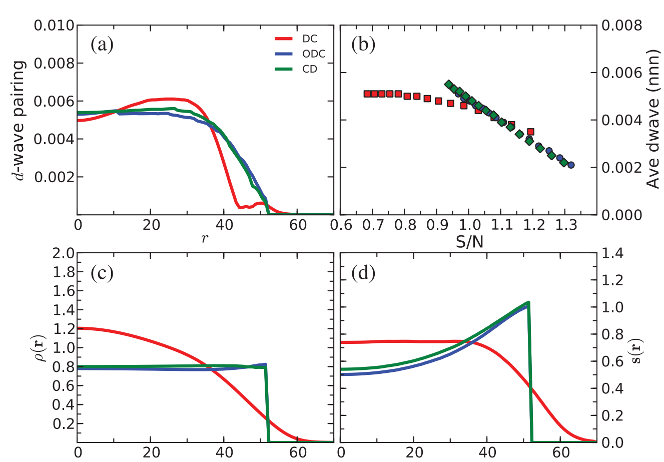


FIG. 4. (Color online) (a) average n.n.n. $d$-wave pairing correlation, (c) density ($\rho$), and (d) entropy per site ($s$) profiles are shown as a function of the distance ($r$) from the trap center for three different trap types: DC, ODC, and constant density (CD) using optimal trap parameters for each type. The average pairing values for CD and ODC traps are 0.0052 and 0.0051, with the DC trap at 0.0046. Entropy per fermion (0.95) and number of fermions (6600) is the same for each trap. Panel (b) shows average $d$-wave response as a function of entropy per fermion ($S/N$) for optimal DC, ODC, and CD traps.

(CD) traps at the same entropy per fermion (0.95) and number of fermions (6600). Optimal parameters obtained for each trap are as follows: DC ($U = 4.5, \mu_0 = 1.5, V_t = 0.00235$), ODC ($U = 3.0, \mu_0 = -1.1, \alpha = 0.00032$), and CD ($U = 3.0, \alpha = 0.00032, \rho = 0.80$).

Looking at the trap profiles, we can see that peak pairing for the DC trap occurs at lattice distances (measured from the center) which correspond to densities between 0.9 and 1.1, but pairing dips outside of this region and falls off rapidly toward the trap edge. The constant density and ODC traps are characterized by larger average pairing values of 0.0052 and 0.0051 (vs 0.0046 for DC). This result can be clearly understood from Fig. 2(c) by observing how the constant density line ($\rho = 0.80$) and ODC path follow the ridge of high $d$-wave pairing response, while the DC trap path cuts through this ridge for only a portion of the trap area. While the pairing difference is not large at this high entropy level, the advantage is expected to grow at lower entropies (see discussion in next section).

Figure 2(c) also emphasizes the narrowness of the optimal $d$-wave response region compared to the wider area of magnetic response seen in Fig. 2(b). This suggests that OLE trap parameters tuned to follow this ridge of high $d$-wave response will increase the potential for observing superconducting order.

## VII. SUMMARY OF TRAP COMPARISONS

Figures 3(b) and 4(b) summarize the results of our trap comparisons by plotting the optimal $\langle m \rangle$ and $\langle p \rangle$ for the different confining schemes against entropy per fermion ($S/N$). In the range of entropy shown, the DC trap produces a larger antiferromagnetic signal than the corresponding ODC trap at the same entropy. On the other hand, while the average $d$-wave pairing correlation in a DC trap flattens at low entropy ($S/N \sim 0.6 - 0.9$), that of a CD or an ODC trap continues to increase as entropy is lowered. Due to the sign problem, we were unable to reach entropy per fermion levels lower than 0.9 for ODC and CD traps, but it is evident from Fig. 4(b) that the $d$-wave response continues to rise as $S/N$ decreases.

## VIII. CONCLUSIONS

We have evaluated several trapping geometries for fermions in a 2D optical lattice. For magnetic properties, the DC trap, which is the common experimental technique used in OLE, continues to be the most promising confinement approach because excess entropy can be stored in its low density wings leaving a low entropy Mott region with large AFM correlations. We have also shown that a more robust signal of $d$-wave pairing is produced with a constant density trap with optimal $\rho \sim 0.80$, where local pairing correlations extend over a significantly greater fraction of sites. We find that ODC closely follows the constant density line shown in Fig. 2.

An important conclusion of our work is that while the search for antiferromagnetic correlations in optical lattices is aided by the inhomogeneous entropy distribution, this is not the case for pairing. The local entropy is not reduced in the vicinity of $\rho = 0.80$, which is best for $d$-wave superconductivity. Thus the same inhomogeneous $s(r)$ which helps the magnetic signal will weaken the pairing signal. This is a further argument for construction of a trap which has constant density. By providing an optimal confinement template for fermions in two dimensions, we anticipate that the results will aid experimenters in determining the physics of the doped Hubbard model.

## ACKNOWLEDGMENTS

We acknowledge financial support from Army Research Office Award No. W911NF0710576 and the Defense Advanced Research Projects Agency Optical Lattice Emulator Program, Army Research Office Grant 56693-PH, National Science Foundation Grant No. OCI-0904972, CNRS-UC Davis EPOCAL LIA joint research grant, and the Department of Energy SciDAC program (Grant No. DOE-DE-FC0206ER25793). This research was supported in part by an allocation of advanced computing resources provided by the National Science Foundation. The computations benefitted from runs on Kraken at the National Institute for Computational Sciences (http://www.nics.tennessee.edu/). We are grateful for inspiration from G. Thorogood.

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