Determinant Quantum Monte Carlo Study of d-wave pairing in the Plaquette Hubbard Hamiltonian

T. Ying\textsuperscript{1}, R. Mondaini\textsuperscript{3,4}, X.D. Sun\textsuperscript{1}, T. Paiva\textsuperscript{2}, and R.T. Scalettar\textsuperscript{4}

\textsuperscript{1}Department of Physics, Harbin Institute of Technology, Harbin 150001, China
\textsuperscript{2}Instituto de Física, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro RJ, Brazil
\textsuperscript{3}Physics Department, The Pennsylvania State University, 104 Davey Laboratory, University Park, Pennsylvania 16802, USA and
\textsuperscript{4}Physics Department, University of California, Davis, California 95616, USA

Determinant Quantum Monte Carlo (DQMC) is used to determine the pairing and magnetic response for a Hubbard model built up from four site clusters- a two dimensional square lattice consisting of elemental 2x2 plaquettes with hopping $t$ and on-site repulsion $U$ coupled by an interplaquette hopping $t' \leq t$. Superconductivity in this geometry has previously been studied by a variety of analytic and numeric methods, with differing conclusions concerning whether the pairing correlations and transition temperature are raised by the inhomogeneous hopping or not. DQMC indicates an optimal $t'/t \approx 0.4$ at which the pairing vertex is most attractive. We contrast our results for this plaquette model with a Hamiltonian which instead involves a regular pattern of site energies whose large site energy limit is the three band CuO$_2$ model, and show the inhomogeneity rapidly, and monotonically, suppresses pairing.

PACS numbers: 71.10.Fd, 02.70.Uu

I. INTRODUCTION

One of the earliest numerical indications of the possibility that an on-site electron-electron interaction $U$ might play a role in novel superconducting materials was the observation of a negative “binding energy” in exact diagonalization studies of the Hubbard Hamiltonian on 2x2 clusters. In this geometry, the ground state energy diagonalization studies of the Hubbard Hamiltonian on the observation of a negative “binding energy” in exact might play a role in novel superconducting materials was.

The observation that the $n$th hopping focused on the “checkerboard Hubbard model” which amount of analytic and numeric attention has been suggested possible relevance of models involving such other geometries, e.g., on one dimensional chains of 2x2 plaquettes with cuprate superconductors,\textsuperscript{10} Pair binding was also studied on larger Hubbard clusters\textsuperscript{11} and on other geometries, e.g., on one dimensional chains of varying length\textsuperscript{12} with three electronic bands\textsuperscript{13} models with intersite interactions\textsuperscript{14} and the strong coupling $t$-$J$ limit\textsuperscript{15,16}.

Following these small cluster studies, a considerable amount of analytic and numeric attention has been focused on the “checkerboard Hubbard model” which consists of a periodic array of 2x2 plaquettes with hopping $t$ and repulsion $U$ connected by a weaker hybridization $t'$. It was suggested that the plaquettes act as centers of attraction, which then drive superconductivity in the extended lattice. This picture provides a ‘local’ counterpart to theories of pairing which focus qualitatively on the exchange of magnetic fluctuations. Perhaps unsurprisingly, the presence of inhomogeneous hoppings introduces new phases to the Mott insulator, antiferromagnetic, and $d$-wave superconductor typically discussed in the uniform $t = t'$ case. Specifically, the quantum numbers and symmetries of the 2x2 plaquette can evolve into a wide variety of ground states when $t'$ is made nonzero.\textsuperscript{12} An additional diagonal hopping can also change the ground state of the 2x2 plaquette building block\textsuperscript{13} and induce new types of crystalline insulators.

A key conceptual question concerns the existence of an ‘optimal inhomogeneity’\textsuperscript{13,14} As pointed out by Tsai and Kivelson\textsuperscript{14} pairing which exists at very weak $t'$ is expected to exhibit a critical temperature $T_c$ which increases as $t'$ grows. If it were the case that $T_c$ is small or zero in the homogeneous model $t' = t$, this necessarily implies a maximal $T_c$ at an intermediate value $0 < t'/t < 1$. Exact diagonalization of 4x4 clusters\textsuperscript{15} indicated that this maximum occurs at $t'/t \approx 0.5$ and $U \approx 8t$. Additional evidence for an optimal inhomogeneity in the plaquette Hubbard model is provided by a contractor-renormalization (CORE) study\textsuperscript{16} where the pair binding energy was found to be maximized in the range $0.5 < t'/t < 0.7$ and $5 < U/t < 8$.

In related work, the density matrix renormalization group method has been used to study a collection of 2x2 plaquettes connected to form a two leg ladder\textsuperscript{20} It was found that, close to half-filling, $U/t \approx 6$ and $t'/t \approx 0.6$ gives the optimal pair binding energy. Although there can be no finite temperature transition in such one-dimensional ladder geometries, an interchain mean field theory suggests that the critical temperature again exhibits an ‘optimal degree of inhomogeneity’ with a maximum occurring at $t' < t$.

There have also been several methods which challenge the idea of an optimal inhomogeneity at intermediate $t'/t$. The central result of a Dynamical Cluster Approximation (DCA) analysis\textsuperscript{11} was that the critical temperature $T_c$ for $d$-wave pairing is maximal for $t'/t = 1$ for interaction strengths $U$ of the order of the bandwidth.
and lattice fillings $\rho \approx 0.9$. That is, inhomogeneity monotonically suppresses superconductivity. The qualitative physical picture behind this conclusion was that inhomogeneities reduce the magnetic contributions to the pairing interaction.\textsuperscript{22,24}

Cellular Dynamical Mean Field Theory (CDMFT) is another approach with which the plaquette Hubbard Hamiltonian has been analyzed.\textsuperscript{25} At weak coupling, inhomogeneity reduces the order parameter for small to intermediate doping, but enhances it at larger doping. For strong coupling, inhomogeneity suppresses pairing for all doping. Overall, the CDMFT results seem consistent with those of the DCA, namely that for inhomogeneity in the nearest-neighbor hopping such as is present in the plaquette Hubbard model, the superconducting order parameter does not exceed that of the uniform system.

The contrasting results between the DMRG+interchain MFT, CORE, and exact diagonalization treatments, and other cases in which optimal inhomogeneity occurs, on one hand, and the DCA, CDMFT methods on the other, provide the motivation for the work described in this manuscript - a study of the plaquette Hubbard Hamiltonian\textsuperscript{26} using the Determinant Quantum Monte Carlo method.\textsuperscript{27,28}

The remainder of this paper is organized as follows: In Sec. II we write down the plaquette Hubbard Hamiltonian and discuss the measurements we use to monitor $d$-wave pairing. We also provide a brief summary of the DQMC algorithm and its limitations. In Sec. III we discuss our results at half-filling and in the doped case. Our central conclusion is that an optimal degree of inhomogeneity does occur in the plaquette Hubbard model, although the largest pairing signal appears to occur at $t'/t \approx 0.4$, a bit less than that reported in other work. However, the sign problem restricts us to higher temperatures than those accessible in the DCA and CDMFT.\textsuperscript{25} Section IV discusses the effect on pairing of another form of inhomogeneity in which the site energies are varied periodically across the lattice. The paper concludes with a summary of our findings.

II. THE PLAQUETTE HUBBARD HAMILTONIAN

The plaquette Hubbard Hamiltonian is

\[ \hat{H} = -t \sum_{(ij) \in P, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) \]
\[ -t' \sum_{(ij) \notin P, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) \]
\[ + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) \]

Here $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) are the usual creation(destruction) operators for fermions of spin $\sigma$ on lattice site $i$. The designations $(ij) \in P$ and $(ij) \notin P$ in the kinetic energy terms convey the fact that hopping $t$ between near neighbor sites $i,j$ on the same plaquette is different from the hopping $t'$ for sites $i,j$ on different plaquettes. This geometry is illustrated in Fig. 1. We have written the interaction term in particle-hole symmetric form, so that $\mu = 0$ corresponds to half-filling. (Note that the Hubbard Hamiltonian with near-neighbor hopping on a bipartite lattice is particle-hole symmetric for any pattern of intersite hoppings $t_{ij}$, and hence, in particular, for the case considered here.)

In the Determinant Quantum Monte Carlo (DQMC) algorithm,\textsuperscript{27,28} the expectation values of observables $\langle A \rangle = \text{Tr} A \exp(-\beta \hat{H})/\text{Tr} \exp(-\beta \hat{H})$ for fermionic Hamiltonians like Eq. 1 are evaluated by discretizing the inverse temperature $\beta$ and rewriting the partition function as a path integral. Replacing the exponential of the interaction terms in the Hamiltonian by a coupling of quadratic fermion operators to a Hubbard-Stratonovich field allows the fermions to be integrated out analytically, leaving a product of fermion determinants (one determinant for each spin species) as the weight to sample the Hubbard-Stratonovich field. Each operator $A$ can then be measured by accumulating appropriate combinations of Green’s functions, the inverse of the matrices whose determinants form the Boltzmann weight. As described further below, the flexibility to alter the order in which the Monte Carlo average is performed and in which the Green’s functions are multiplied can be used to control which many body effects are included in the expectation value, and hence to isolate the pairing vertex.

The central limitation to the DQMC algorithm is the sign problem,\textsuperscript{29} which arises when the product of determinants becomes negative. This will restrict the temperatures accessible in the study reported here, and, as a consequence, temper our ability to make conclusive statements about the effect of inhomogeneity in the case when the system is doped. At half-filling, because spatial variations in the hopping do not destroy particle-hole symmetry, there is no sign problem and DQMC
can access the ground state for any \( t'/t \). Off half-filling data for the average sign \( \langle S \rangle \) are given in Fig. 2. \( \langle S \rangle \) is relatively weakly dependent on \( t'/t \). The lowest accessible temperature is around \( T/t \sim 1/5 \) for the entire range \( 0 < t' < 1 \), although simulations become somewhat more difficult as \( t'/t \) decreases. It is possible to get accurate data for certain quantities, like the density, for quite small values of \( \langle S \rangle \). However for more complex quantities like magnetic and pair correlations at large distances, if reasonable accuracy (statistical error bars less than 10%) is desired, then \( \langle S \rangle \gtrsim 0.3 \) is needed. \( \langle S \rangle \) is roughly the same for the two densities \( \rho = 0.875 \) and \( \rho = 0.774 \) shown. For \( \rho = 0.500 \), however, \( \langle S \rangle \) is better behaved (not shown) and reliable averages can be obtained for temperatures as low as \( T/t = 1/16 \), for several values of \( t'/t \).

The spectrum of the \( U = 0 \) hopping Hamiltonian for an isolated 2x2 plaquette consists of four energy levels, \( E = -2t, 0, 0, 2t \). As \( t' \) is turned on, these discrete levels broaden until they finally merge into the 2D square lattice density of states \( N(E) \) at \( t' = t \). This evolution is shown in Fig. 3. At half-filling, where \( E_{\text{Fermi}} = 0 \), and for small dopings, \( N(E_{\text{Fermi}}) \) is enhanced by inhomogeneity. In principle this might lead to a greater tendency to ordered phases, including superconducting ones, although the possibly competing effect of inhomogeneity on the interaction vertex must also be considered.\(^{23}\)

For large inhomogeneity \( (t'/t < 0.5) \) the discrete 2x2 eigen-levels are not sufficiently broadened by \( t' \) to coalesce into a single band, and the noninteracting system is a band insulator at \( \rho = 0.5 \) and \( \rho = 1.5 \). Figure 4 shows QMC data for \( \rho(\mu) \) at interaction strengths \( U/t = 2 \) and \( U/t = 4 \) and weakly coupled plaquettes \( t'/t = 0.2 \). There is a band gap evident at \( \rho = 0.5 \) (and also, due to particle-hole symmetry at \( \rho = 1.5 \), not shown). Non-zero \( U/t \) is also seen to cause an insulating gap to develop at half-filling, \( \rho = 1 \). This is a dramatic change from the noninteracting limit, since it represents the suppression of the large peak in \( N(E) \) at \( E = 0 \) in Fig. 3. The development of this gap, even though \( U/t \) is much less than the bandwidth, is associated with the onset of long range antiferromagnetic order, as we shall see in the next section. Notice that reasonable data can be obtained for the density even at \( U/t = 4, \beta t = 16 \). This, however, is not true for more complicated spin and pair correlations.

The equal time spin correlation function and magnetic structure factor are given by,

\[
S^+(q_x, q_y) = \frac{1}{N} \sum_{i,j} c_{\text{spin}}(\vec{r}) e^{i\vec{q} \cdot \vec{r}}
\]

(2)

with an analogous expression for \( S^{zz}(q_x, q_y) \). In the homogeneous system it is known that at \( T = 0 \) and at half-filling the 2D Hubbard Hamiltonian possesses long range magnetic order.\(^{24,25}\) That is, the spin-spin correlations \( c_{\text{spin}}(\vec{r}) \) in real space approach a nonzero value asymptotically as \( |\vec{r}| \to \infty \). On finite sized lattices, this is established by an appropriate scaling of
the structure factor with lattice size.\textsuperscript{33}

As with magnetic order, a tendency to $d$-wave pairing can be examined via the asymptotic behavior of equal time correlations,

$$c_{d\text{pair}}(\vec{r}) = \langle \Delta_d \vec{r}_0 + \vec{r} \Delta_d \vec{r}_0 \rangle$$

However, a more sensitive measurement, and one which makes better contact with previous DCA work,\textsuperscript{21} is the $d$-wave pairing susceptibility,

$$c_{d\text{pair}}(\vec{r}, \tau) = \langle \Delta_d \vec{r}_0 + \vec{r}(\tau) \Delta_d \vec{r}_0(\tau) \rangle$$

$$\Delta_d^{\uparrow \downarrow}(\tau) = e^{-\beta H_0} \Delta_d^{\uparrow \downarrow}(0) e^{-\tau H}$$

$$P_d = \sum_{\vec{r}} \int_0^\beta c_{d\text{pair}}(\vec{r}, \tau) \, d\tau \quad \text{(4)}$$

$P_d$ is a preferred diagnostic of superconductivity, especially if the sign problem precludes going to low temperatures, because it allows for a comparison between the fully dressed susceptibility and the uncoupled susceptibility $P_d$, and hence an indication of pairing even when only short range order is present.\textsuperscript{33} The technical distinction between $P_d$ and $\overline{P}_d$ in a DQMC simulation is that when the expectation value of the four fermion terms in Eq. 4 is evaluated, the Green’s functions obtained by the Wick contractions are first multiplied together and then averaged to obtain $P_d$, whereas for $\overline{P}_d$, the Green’s functions are first averaged and then multiplied. In $\overline{P}_d$ the effect of the interactions is only to dress the individual single particle propagators, while $P_d$ includes all interaction effects.\textsuperscript{33}

This distinction allows us to extract the interaction vertex $\Gamma_d$ from $P_d$ and $\overline{P}_d$:

$$\Gamma_d = \frac{1}{P_d} - \frac{1}{\overline{P}_d} \quad \text{(5)}$$

If $\Gamma_d \overline{P}_d < 0$, the associated pairing interaction is attractive. More precisely, Eq. 5 can be re-written as,

$$P_d = \frac{\overline{P}_d}{1 + \Gamma_d \overline{P}_d} \quad \text{(6)}$$

so that $\Gamma_d \overline{P}_d \to -1$ signals a superconducting instability.

\section{III. RESULTS}
\subsection{A. Half-Filling}

Our central interest is in the doped lattice, where antiferromagnetism might potentially give way to $d$-wave pairing. However, we begin by briefly showing results at

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4}
\caption{(Color online) Density as a function of chemical potential for an 8x8 lattice at $t'/t = 0.2$. The band gaps evident in the $U = 0$ density of states at $\rho = 0.5$ and $\rho = 1.5$ (Fig. 3) persist at weak to intermediate coupling $U/t = 2-4$ shown here. (Since $\rho$ is particle-hole symmetric we focus on $\rho \leq 1$.) However the interactions also drive the formation of an insulating gap at $\rho = 1$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5}
\caption{(Color online) Spin (a) and charge (b) correlations along an intraplaquette bond (black squares), interplaquette bond (red circles), and along the diagonal of the plaquette (blue triangles). Here $\rho = 1$, $U/t = 4$, and $\beta t = 5$. The lattice is 8x8.}
\end{figure}
The pairing vertex and the uncorrelated susceptibility. 

\[
\delta c_{\text{spin}}(\vec{r}) = \begin{cases} 
\frac{c_{\text{spin}}^{t=0.8}(\vec{r}) - c_{\text{spin}}^{t=1.0}(\vec{r})}{c_{\text{spin}}^{t=0.8}(\vec{r}) + c_{\text{spin}}^{t=1.0}(\vec{r})} 
\end{cases}
\]

Panel (a) has \( \vec{r} \) along the \((1,0)\) direction, and panel (b) along the \((1,1)\) direction. With the exception of the correlation for spins which are first neighbors in different plaquettes, all values of \( \vec{r} \) show an increase, \( \delta c_{\text{spin}}(t'=0) \) is small further informs us that the effect is not just due to a trivial change in the local moment.

**B. The doped lattice**

After this brief synopsis of results at \( \rho = 1 \), we turn to the case when the filling is incommensurate, the situation of most interest to understanding cuprate superconductivity.

Fig. 8 shows the same spin correlations as in Fig. 5(a), but for \( \rho = 0.500 \) (a), \( \rho = 0.774 \) (b) and \( \rho = 0.875 \) (c). The NN spin correlations exhibit the expected evolution with density- they are largest at \( \rho = 1.000 \) (Fig. 5(a)), and decrease as we move away from half-filling. Similar to what happens at half-filling, the NNN spin correlation inside a plaquette is positive for \( \rho = 0.875 \), again as expected for antiferromagnetism, but decreases with growing \( t' \). With decreasing density the behavior for this quantity changes: for \( \rho = 0.774 \), \( c_{\text{spin}}(1,1) \) is essentially zero for all \( t'/t \). For \( \rho = 0.500 \), however, it is negative and increases in magnitude as the connection between the plaquettes is reduced. This later result can be understood when we recall that at this

![Graph showing \( \Gamma P_{d} \) and \( S \) as functions of \( t'/t \).](image)
density the system has 2 fermions in every plaquette on average. The configuration which minimizes the kinetic energy and the local repulsive interaction is a singlet state with spins residing on NNN neighbors. In this case the NNN correlation becomes negative. This effect is enhanced as $t'/t$ is smaller.

Figure 7 shows short-range $d$-wave pair correlations for the same densities as Fig. 8. Contrary to what is observed for spin correlations, both NN and NNN pairing correlations increase with decreasing density.

Having described the short range, real space correlations, we now turn to more sensitive magnetic and pairing structure factors and susceptibilities. The latter especially has an enhanced signal since it is sensitive to the build-up of correlations in the imaginary time direction. The magnetic structure factor dependence on $t'/t$ and $q_x,q_y$ for three different dopings on an 8x8 lattice at inverse temperature $\beta t = 5$ is shown in Fig. 10. Near half-filling ($\rho = 0.875, 0.774$) $S(q_x,q_y)$ is peaked at $(\pi,\pi)$, indicating the dominance of antiferromagnetic correlations. At $\rho = 0.875$ the AF peak substantially increases as $t' \to t$, with a concomitant reduction in $S$ at other momenta. Presumably these effects would become larger at lower $T$. However, $\beta t \approx 5$ is the limit accessible to DQMC owing to the sign problem. For lower densities, $S(q_x,q_y)$ is rather insensitive to $t'$.

There is a substantial difference in scale of the antiferromagnetic structure factor: $S_{AF} = S(\pi,\pi) \sim 1$ in the doped lattice, whereas at half-filling, $S_{AF} \sim 10$ (Fig. 9). This arises both from the rapid suppression of antiferromagnetic order with doping in the square lattice Hubbard mode, and also because of the lower temperatures that can be reached at $\rho = 1$ ($\beta t \sim 10 - 16$) compared to $\rho \neq 1$ ($\beta t \sim 5$).

At $\rho = 0.875$ the overall evolution with $t'$ of the antiferromagnetic structure factor $S(\pi,\pi)$ in Fig. 10 is consistent with that found in 19. That is, $S(\pi,\pi)$ increases monotonically with $t'$ and is maximal at $t' = t$. However, the two results appear to differ in the finer details. Specifically, the CORE study indicates that the staggered magnetic order parameter is roughly constant for $0 < t'/t < 0.5$, and then increases rather abruptly at $t'/t \approx 0.6$. This is mirrored in an increase in the number of magnons, a phenomenon to which the appearance of a maximum in the pair binding energy is attributed. In contrast, our DQMC data appear to indicate a more immediate rise in $S(\pi,\pi)$ as $t'$ grows from zero. A possible origin of the difference is that our work is at finite temperature, whereas the CORE study is in the ground state. Indeed, at half-filling it is known that $S(\pi,\pi)$ does not reach its low $T$ values until $T \lesssim 0.08t$, temperatures which are not accessible when the system is doped, due
The choice $\rho = 0.5$ does however improve the average sign enough to see the $t'/t$ evolution of $d$-wave pairing, which we established to have an optimal inhomogeneity at half-filling. Fig. 12 (a) shows $\Gamma_d \bar{P}_d$ versus $T$ for different $t'/t$. As at $\rho = 1$, there is evidence for an optimal inhomogeneity: in the uniform case $\Gamma_d \bar{P}_d$ versus $T$ is almost temperature independent and is also small, $|\Gamma_d \bar{P}_d| \lesssim 0.01$. As inhomogeneity is turned on to $t'/t \sim 0.5$, $|\Gamma_d \bar{P}_d|$ increases by almost an order of magnitude (although it is still far from the $\Gamma_d \bar{P}_d = -1$ criterion for a transition. Further increase of the inhomogeneity to $t'/t < 0.5$ decreases $|\Gamma_d \bar{P}_d|$. The same optimum $t'/t \sim 0.5$ can be seen for $\rho = 0.774$, as shown in Fig. 12 (b).

Early in DQMC studies of the homogeneous square
lattice it was established that $d$-wave pairing is the dominant superconducting instability. This conclusion is not altered by $t' \neq t$. Fig. 13 shows results like Fig. 11 for $s$ and extended $s$ ($s^*$) symmetry channels. The correlations are obtained in a similar fashion as in the $d$-wave case but the associated phases in Eq. 4 are positive. For the $s$ symmetry the pairs are created and destroyed locally \( \left( \Delta_{s,r} = c_{r+\hat{x}}^\dagger c_{r}^\dagger + c_{r-\hat{x}}^\dagger c_{r}^\dagger \right) \), whereas in the extended one they all enter with the same phase sign \( \left( \Delta_{s^*,r} = c_{r+\hat{x}}^\dagger c_{r}^\dagger + c_{r-\hat{x}}^\dagger c_{r}^\dagger \right) \). While $s$-wave symmetry produces only repulsive interactions, some parameters in the $s^*$-wave case exhibit attraction. Nonetheless it is much smaller in magnitude than $d$-wave symmetry.

![Figure 11](image1.png)

**FIG. 11:** (Color online) Dependence of the pairing vertex on $t'/t$ away from half filling. All densities appear to show a maximum of $\Gamma_d^d$ at intermediate $t'/t$. The lattice size is $8x8$, $U/t = 4$ and $\beta t = 5$. Also included for comparison the $\beta t = 7$ in the $\rho = 0.500$ case.

![Figure 12](image2.png)

**FIG. 12:** (Color online) The evolution of $\Gamma_d^d$ with $T/t$ for $\rho = 0.500$ (a) and $\rho = 0.774$ (b). The plots emphasize the existence of an optimal degree of inhomogeneity. Here the lattice size is $8x8$ and $U/t = 4$

![Figure 13](image3.png)

**FIG. 13:** (Color online) Same as Fig. 11 but now comparing the interaction vertex times the uncorrelated susceptibility for two other symmetry channels: $s$ in (a) and $s^*$ in (b). While in the former all densities result in a repulsion between the pairs for the whole range of $t'/t$ studied, in the latter depending on the specific parameters the pairing turns attractive but is substantially smaller in magnitude in comparison to the $d$-wave symmetry channel.

### IV. CHECKERBOARD HUBBARD MODEL

The nature of pairing in models with other sorts of inhomogeneities, e.g. built of two site dimers rather than four site clusters\(^{23}\) modulated by different site potentials\(^{30}\) or consisting of lines of different chemical potentials, alternating between half-filled antiferromagnetic stripes and doped stripes has also been explored\(^{31}\). In this section we examine the effects on pairing of an inhomogeneity pattern in which the local energies on a regular pattern of sites is raised by an amount $V_0$. That is, we add a term $H' = V_0 \sum_{l \in A, \sigma} n_{l\sigma}$ to the Hubbard Hamiltonian Eq. 1 with $t' = t$. The collection $A$ consists of a fraction $f$ of the lattice sites.
FIG. 14: (Color online) Checkerboard geometry, in which a fraction $f$ of the sites, displayed in a checkerboard pattern, has on site energy raised by $V_0 \neq 0$. Panel (a) shows the $f = 1/4$ lattice and (b) the $f = 1/2$ one, for 8x8 systems.

FIG. 15: (Color online) Product of interaction vertex $\Gamma_d$ and uncorrelated susceptibility $\bar{\Gamma}_d$ for a Hubbard model with an alternating pattern of site energies. (See Fig. 14(a).) The vertex is weakly attractive for the homogeneous case, $V_0 = 0$, but becomes repulsive for $V_0 \gtrsim 1$. Here the lattice size is 16x16, filling $\rho = 0.774$ in (a) and $\rho = 0.875$ in (b), and interaction strength $U = 4t$.

This geometry is illustrated in Fig. 14 for $f = 1/4$ (a) and $f = 1/2$ (b), the two cases analyzed here.

One motivation for considering this particular pattern with $f = 1/4$ is that in the limit $V_0 \to \infty$ the lattice maps onto the ‘three band’ Hamiltonian sometimes used to model the CuO$_2$ plane of the cuprate superconductors (with, however, the choice of equal copper $d$ and oxygen $p$ energies.) The red sites without any blue neighbors are like the Cu atoms, while the red sites with two blue neighbors represent the O sites which link the Cu. Thus this model makes partial contact with earlier studies of binding on CuO$_2$ clusters in the limit $\epsilon_{pd} = 0$. Another point of contact of this model is to other inhomogeneity patterns which share an $f = 1/4$ proportion of sites with raised on-site energy, for example 21 in which a pattern of stripes was shown to enhance $d$-wave pairing away from half-filling.

Results for this site-energy inhomogeneous geometry ($f = 1/4$) are shown in Fig. 15(a). In stark contrast to the plaquette model and to the striped $V_0$ model 21 $\Gamma_d \bar{\Gamma}_d$ becomes positive when $V_0$ is turned on: the $d$-wave pairing vertex is made repulsive. As with the plaquette Hamiltonian of the previous sections, we are interested in how the dependence of pairing on inhomogeneity is affected by the density. To this end we show, in Fig. 15(b), the same quantity but with $\rho = 0.875$. This data is consistent with the previous density, and we conclude that this form of site energy inhomogeneity competes destructively with superconductivity.

Finally, we consider a pattern of inhomogeneity with $f = 1/2$, (see Fig. 14(b).) Fig. 16 demonstrates the effect of $V_0$ is monotonic and mimics to superconductivity.

V. CONCLUSIONS

Study of the effect of inhomogeneities on superconductivity has been a focus of much computational effort on the Hubbard and $t – J$ models over the last decade. One branch of effort has explored models where inhomogeneity is included in the Hamiltonian itself. Other work concerns the
question of inhomogeneity which arises spontaneously in a translationally invariant Hamiltonian. The plaquette Hubbard model has been a natural candidate of interest since it seems to contain the nascent element, a substantial binding energy, in its building blocks.

We have shown here that DQMC indicates that the most sensitive of measurements of $d$-wave pairing yields an ‘optimal degree of inhomogeneity’. That is $\Gamma_{d'}^d$ at $t'/t = 0$ or $t'/t = 1$. This result agrees qualitatively with some past numeric work (differing in the precise optimal $t'/t$), but is in disagreement with several of the most powerful computational methods available for these sorts of problems. Although the indications in our work are that the optimal inhomogeneity develops further as $T$ is lowered, the sign problem prevents us from going to very low temperatures.

Acknowledgements: This work was supported by the National Key Basic Research Program of China, Grant No. 2013CB328702, by DOE [de-na0001842], and by the Office of the President of the University of California. Support from CNPq and FAPERJ (TP and RM) is gratefully acknowledged.

1 D.J. Scalapino and S.A. Trugman, Philos. Mag. B 74, 607 (1996).
2 J.A. Riera and A.P. Young, Phys. Rev. B 39, 9697 (1989).
3 E. Dagotto, A. Moreo, R.L. Sugar, and D. Toussaint, Phys. Rev. B 41, 811 (1990).
4 R.M. Fye, M.J. Martins, and R.T. Scalettar, Phys. Rev. B 42, 6809 (1990).
5 J.E. Hirsch, S. Tang, E. Loh, and D.J. Scalapino, Phys. Rev. Lett. 60, 1668 (1988).
6 C.A. Balseiro, A.G. Rojo, E.R. Gagliano, and B. Alascio, Phys. Rev. B 38, 9315 (1988).
7 J.E. Hirsch, E. Loh, and D.J. Scalapino, and S. Tang, Phys. Rev. B 39, 243 (1989).
8 J. Callaway, D.P. Chen, D.G. Kanhere, and Q. Li, Phys. Rev. B 42, 465 (1990).
9 E. Kaxiras and E. Manousakis, Phys. Rev. B 38, 866 (1989).
10 J. Bonca, P. Prelovsek, and I. Sega, Phys. Rev. B 39, 7074 (1989).
11 Y. Hasegawa and D. Poilblanc, Phys. Rev. B 40, 9035 (1989).
12 H. Yao, W-F. Tsai, and S.A. Kivelson, Phys. Rev. B 76, 161104(R) (2007).
13 H. Yao and S.A. Kivelson, Phys. Rev. Lett. 105, 166402 (2010).
14 E. Arrigoni, E. Fradkin, and S.A. Kivelson, Phys. Rev. B 69, 214519 (2004).
15 I. Martin, D. Podolsky, and S.A. Kivelson, Phys. Rev. B 72, 060502(R) (2005).
16 S.A. Kivelson and E. Fradkin, in Handbook of High-Temperature Superconductivity, edited by J.R. Schrieffer and J.S. Brooks (Springer, New York, 2007).
17 W.F. Tsai and S.A. Kivelson, Phys. Rev. B 73, 214510 (2006).
18 W.-F. Tsai, H. Yao, A. Lauchli, and S. A. Kivelson, Phys. Rev. B 77, 214502 (2008).
19 S. Baruch and D. Orgad, Phys. Rev. B 82, 134537 (2010).
20 G. Karakostantakis, E. Berg, S.R. White, and S.A. Kivelson, Phys. Rev. B 83, 054508 (2011).
21 D.G.S. Doluweera, A. Macridin, T. A. Maier, M. Jarrell, and T. Pruschke, Phys. Rev. B 78, 020504(R) (2008).
22 T. A. Maier, M. Jarrell, and D. J. Scalapino, Phys. Rev. B 74, 094513 (2006).
23 T.A. Maier, M. Jarrell, and D.J. Scalapino, Phys. Rev. B 75, 134519 (2007).
24 T.A. Maier, A. Macridin, M. Jarrell, and D.J. Scalapino, Phys. Rev. B 76, 144516 (2007).
25 S. Chakraborty, D. Sénéchal, and A.-M.S. Tremblay, Phys. Rev. B 84, 054545 (2011).
26 It is worth noting that there is a considerable literature on another model sometimes also referred to as the “checkerboard Hubbard Hamiltonian” (or “2D pyrochlore” Hamiltonian) [29][30]. In this model, hopping is present along the diagonal of alternating plaquettes of the square lattice Hubbard Hamiltonian. One key question is whether a spin liquid phase in which there is no symmetry breaking emerges due to the frustration, or whether the ground state retains some sort of translation-invariance-breaking or exotic pairing order. The model considered in [13] contains elements both of a Hamiltonian built up of linked plaquettes and the frustrating effects of diagonal hopping.
27 R. Blankenbecler, D.J. Scalapino, and R.L. Sugar, Phys. Rev. D 24, 2278 (1981).
28 S.R. White, D.J. Scalapino, R.L. Sugar, E.Y. Loh Jr., J.E. Gubernatis, and R.T. Scalettar, Phys. Rev. B 40, 506 (1989).
29 T. Yoshioka, A. Koga, and N. Kawakami, Phys. Rev. B 78, 155113 (2008).
30 F. Trouseau, D. Poilblanc, and R. Moessner, Phys. Rev. B 78, 195101 (2008).
31 D. Poilblanc, K. Penc, and N. Shannon, Phys. Rev. B 75, 220503(R) (2007).
32 H.X. Huang, Y.Q. Li, J.Y. Gan, Y. Chen, and F.C. Zhang, Phys. Rev. B 75, 184523 (2007).
33 M. Indergand, C. Honerkamp, A. Läuchli, D. Poilblanc, and M. Sigrist, Phys. Rev. B 75, 045105 (2007).
34 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).
35 J.E. Hirsch, Phys. Rev. B 31, 4403 (1985).
36 J.E. Hirsch and S. Tang, Phys. Rev. Lett. 62, 591 (1989).
37 C.N. Varney, C.R. Lee, Z.J. Bai, S. Chiesa, M. Jarrell, and R. T. Scalettar, Phys. Rev. B 80, 075116 (2009).
38 D. A. Huse, Phys. Rev. B 37, 2380 (1988).
39 S.R. White, D.J. Scalapino, R.L. Sugar, N.E. Bickers, and R.T. Scalettar, Phys. Rev. B 39, 839 (1989).
40 S. Okamoto and T.A. Maier, Phys. Rev. B 81, 214525 (2010).
41 R. Mondaini, T. Ying, T. Paiva, and R.T. Scalettar, Phys. Rev. B 86, 184506 (2012).