

## Realizing the Strongly Correlated $d$ -Wave Mott-Insulator State in a Fermionic Cold-Atom Optical Lattice

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We show that a new state of matter, the  $d$ -wave Mott-insulator state ( $d$ -Mott state) (introduced recently by [H. Yao, W. F. Tsai, and S. A. Kivelson, Phys. Rev. B **76**, 161104 (2007)]), which is characterized by a nonzero expectation value of a local plaquette operator embedded in an insulating state, can be engineered using ultracold atomic fermions in two-dimensional double-well optical lattices. We characterize and analyze the parameter regime where the  $d$ -Mott state is stable. We predict the testable signatures of the state in the time-of-flight measurements.

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Experimental realizations of degenerate Bose [1,2] and Fermi gases [3–6] in cold-atom optical lattices have led to increasing interaction between the atomic and condensed matter physics communities. In fact, these atomic systems have become a proverbial “playground” where, in principle, custom Hamiltonians [7–9] can be made to order, enabling optical lattice emulations of strongly correlated condensed matter phenomena. Particularly exciting, in this context, is the creation of a fermionic Hubbard model in ultracold atomic systems, since the Hubbard model is a paradigm for theoretical studies of strong correlations. The two-dimensional fermionic Hubbard model, a model woefully difficult to “solve,” is of great interest since it is thought to hold the key to understanding high-temperature (high- $T_C$ ) superconductivity [10]. In fact, the cold-atom systems allow for versatile tuning of the Hamiltonian parameters where the hopping (or tunneling) matrix element between nearest neighbor sites (through laser intensity tuning), the on-site interaction between particles (from attractive to repulsive by tuning the Feshbach resonance), and the dimensionality (from one to three) of the model can all be varied and controlled [7]. Such versatility in tuning the Hamiltonian makes cold-atom systems particularly attractive in studying novel quantum phases and transitions between them.

The possible  $d$ -wave character of the ground state in the Hubbard model is an important concept in relation to the high- $T_C$  cuprate superconductors [10]. Studying the Hubbard model experimentally in the cold atomic gases could, in principle, be an effective and accurate analog simulation of high- $T_C$  superconductivity. Eventually it would be very important to test whether or not the fermionic Hubbard model, in its full generality, allows for  $d$ -wave superfluidity [11–13], a controversial conjecture not yet settled theoretically. In this Letter, we study the model in a controlled limit in which there is (i) an exactly solvable point where a true new state of matter, the so-called  $d$ -Mott state recently discovered by Yao, *et al.* [14] exists as the ground state of the checkerboard Hubbard

model (see below), and (ii) a parameter which can be varied to destroy the  $d$ -Mott state. The  $d$ -Mott state [14] is a special Mott insulating state with a nonzero expectation value ( $-1$ ) of a local plaquette operator,  $D_p$  (see below), which cyclically rotates the sites by an angle  $\pi/2$ . In other words, the state is an insulator with a local plaquette  $d$ -wave symmetry—in analogy with the  $d$ -wave superconductor—characterized by a nonzero expectation value  $\langle D_p \rangle$ . Realizing this state in an optical lattice has its own intrinsic appeal because it is a true new state of matter not adiabatically connected to any other known insulating states [14]. Furthermore, since this is the ground state arising out of an exact solution of the Hubbard model in a controlled limit, it would serve as an important benchmark for the accuracy of experiments aimed at studying the general Hubbard model. For this purpose, we propose and analyze how the distinctive signatures of the  $d$ -Mott state could be observed in the usual time-of-flight measurements. An alternative proposal was provided in Ref. [14].

We consider a system of fermionic atoms ( $^{40}\text{K}$ ) where the two atomic internal hyperfine states,  $|F = 9/2, m_F = -9/2\rangle$  and  $|F = 9/2, m_F = -7/2\rangle$ , are taken as the effective spin states  $\sigma = \uparrow, \downarrow$ . The atoms are loaded into a two-dimensional superlattice, produced by superimposing a long and a short period lattice in the  $x$ - and  $y$ -direction such that an array of square plaquettes is created [15,16]. The dynamics of the atoms can be described by the so-called checkerboard Hubbard model [17] defined as

$$H = - \sum_{\mathbf{r}\delta\sigma} t_{\mathbf{r}}(\delta) c_{\mathbf{r}+\delta\sigma}^{\dagger} c_{\mathbf{r}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}. \quad (1)$$

Here,  $c_{\mathbf{r}\sigma}$  ( $c_{\mathbf{r}\sigma}^{\dagger}$ ) is the particle destruction (creation) operator at lattice site  $\mathbf{r}$  with spin (or magnetic sublevel)  $\sigma$ ,  $t_{\mathbf{r}}(\delta)$  is the hopping amplitude for a particle at site  $\mathbf{r}$  hopping to site  $\mathbf{r} + \delta$ , where site  $\mathbf{r} + \delta$  is a nearest neighbor site,  $U$  is the usual on-site interaction energy, and  $n_{\mathbf{r}\sigma} = c_{\mathbf{r}\sigma}^{\dagger} c_{\mathbf{r}\sigma}$  is the number operator. The checkerboard Hubbard model is defined by choosing  $t_{\mathbf{r}}(\delta) = t$  when  $\delta$  connects sites within

a square plaquette, and  $t_r(\delta) = t'$  when  $\delta$  connects sites between two neighboring square plaquettes; see Fig. 1.

When  $t' = 0$  the ground state of this model can be obtained exactly for all  $U/t$  and all band fillings or densities (dopings) by solving the single plaquette problem exactly (either by brute force [18], Bethe ansatz [19]—four-site plaquette is a one-dimensional ring with four sites—or through numerical exact diagonalization) and constructing the full many-plaquette state as a product state of the plaquette basis states. At exactly half filling (or zero doping, the case considered throughout this work), the ground state for  $U/t > 0$  is an insulator with  $d$ -wave symmetry on the plaquette, the so-called  $d$ -Mott state [14]: the plaquette state is odd under  $\pi/2$  rotations about the plaquette center.

To measure the symmetry characteristic of the  $d$ -Mott state on a plaquette we propose an operator,  $D_P$ , which, when operating on a state, rotates a plaquette by  $\pi/2$  about its center or, alternatively, translates each particle by one site along the four-site “ring.” More concretely, for a particular basis state for demonstrative purposes, the single four-particle four-site plaquette [such as the lattice labeled in Fig. 1(b)] occupation could be  $|n_{1\uparrow}n_{2\downarrow}n_{3\uparrow}n_{4\downarrow}; n_{1\downarrow}n_{2\uparrow}n_{3\downarrow}n_{4\uparrow}\rangle = |1100; 0110\rangle$  where sites 1 and 2 are occupied with spin-up particles and 2 and 3 are occupied with spin-down. The result of operating  $D_P$  on this state is  $D_P|1100; 0110\rangle = |0110; 0011\rangle$ . The particle at site 1 moves to 2,  $2 \rightarrow 3$ ,  $3 \rightarrow 4$ , and  $4 \rightarrow 1$  (the last through periodic boundary conditions on the plaquette). It is easy to see that the possible eigenvalues of  $D_P$  are  $\pm 1$ ,  $\pm i$  since  $(D_P)^4 = 1$ .

For  $t' = 0$  and  $U/t = 0$  the ground state is six-fold degenerate and the operation of  $D_P$  yields  $\pm 1$  or  $\pm i$  for each degenerate ground state. When  $t' = 0$  and  $U/t > 0$ , the degeneracy is broken and a gap  $\Delta$  opens up. The operation of  $D_P$  onto the ground state now yields an eigenvalue equal to  $-1$  indicating the existence of  $d$ -wave symmetry—the state has a nonzero value of the  $d$ -Mott operator  $\langle D_P \rangle$ . In Fig. 2, we plot the gap  $\Delta$  with

respect to  $U/t$ . The gap is zero for  $U = 0$  due to the degeneracy of the ground state while with finite  $U$  the degeneracy is lifted and the gap becomes nonzero. However, the gap also approaches zero in the limit  $U/t \rightarrow \infty$  where there is no phase coherence between the atoms at different sites and the ground state is again degenerate. At a finite  $U/t \approx 6$ , the gap is maximum.

We now consider what happens when  $t' \neq 0$ . An important point to note is that  $D_P$  does not commute with the Hamiltonian for  $t' \neq 0$ , therefore eigenstates of  $H$  will not be eigenstates of  $D_P$ , although  $H$  retains a global  $C_4$  symmetry about the center of any one plaquette. However, there are clearly defined regimes for nonzero values of  $t'$ . As mentioned, for  $t' = 0$  and  $U/t > 0$ , the ground state is gapped and it is an eigenstate of  $H$  and  $D_P$  (with eigenvalue  $-1$ ). For  $t' \ll \Delta$  the ground state is approximately a product state of single plaquette ground states and, hence, remains approximately a simultaneous eigenstate of  $H$  and  $D_P$  (by this we mean that the ground state will have the largest amplitude from basis states that are  $D_P$  eigenstates with eigenvalue  $-1$ ). Thus, it is conceivable that the average value of  $D_P$  for any given plaquette will continue to be nonzero and close to  $-1$  for a nonzero range of  $t'$ . On the other hand, when  $t' \sim t$ , the Hamiltonian is approximately the standard Hubbard model. Thus, the ground state is an essentially equal superposition of  $D_P$  eigenstates, so one expects the value of  $\langle D_P \rangle$ , for any given plaquette, to be zero, since  $1 + (-1) + i + (-i) = 0$ .

The question now becomes exactly what happens for  $U/t > 0$  and  $t' \approx \Delta$  when the particles are first able to hop to the neighboring plaquettes. To answer this question we exactly diagonalize  $H$  for eight particles on an eight-site square lattice ladder with periodic boundary conditions in the “y”-direction depicted in Fig. 1(b) and vary both  $U/t$  and  $t'/t$  from zero to  $t'/t = 1$  and beyond. (Note that a fully periodic system—torus—requires 16 sites with a quite large Hilbert space— $\sim 100$  million states—which is not necessary for establishing the qualitative and semi-quantitative conclusions presented here.) The  $d$ -Mott char-

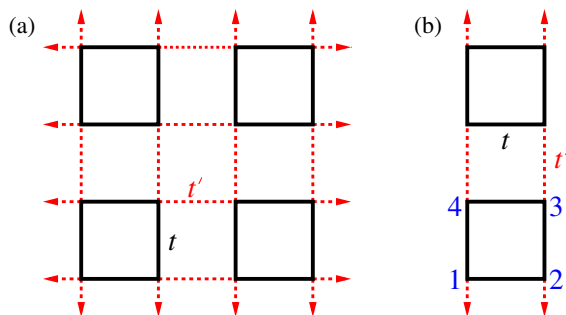


FIG. 1 (color online). (a) Two-dimensional checkerboard Hubbard model. Solid (dashed) bonds represent hopping amplitudes  $t$  ( $t'$ ). (b) “Ladder” cluster we exactly diagonalize with periodic boundary conditions imposed in the “y”-direction and open boundary conditions in the “x”-direction. The numbers label the sites of a single plaquette.

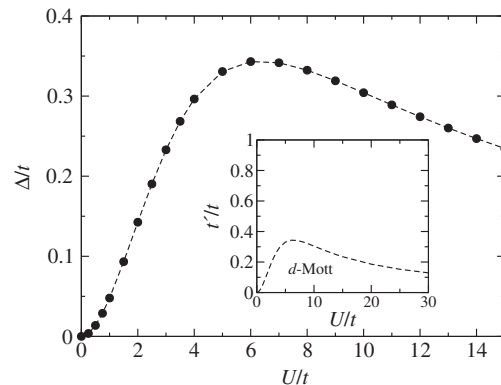


FIG. 2. The gap  $\Delta$  as a function of  $U/t$  for a single plaquette ( $t'/t = 0$ ). The inset shows, approximately, the region in  $(U/t)$ - $(t'/t)$  space where the  $d$ -Mott state is expected to exist.

acter is examined by calculating the average  $\langle D_P \rangle$ . In Fig. 3 we plot  $\langle D_P \rangle$  as a function of  $t'/U$  (left panel) and  $t'/\Delta$  (right panel) for various values of  $U/t$  (weakly to strongly interacting). From the left panel we see that the behavior is largely universal when plotted versus  $t'/U$  and the value drops well below  $-1$  for  $t' \approx t$ . However, the physics is better elucidated in the right panel. Here it is clearly seen that once  $t'$  becomes equal to, and exceeds, the single plaquette gap  $\Delta$  the  $d$ -Mott order is quickly lost. Thus, the optimal parameter regime for observing the  $d$ -Mott state is at  $U/t \approx 6$ , where the gap  $\Delta$  reaches the maximum and the  $d$ -Mott state, with a nonzero expectation value of the local plaquette operator  $D_P$ , is most stable against the interplaquette coupling  $t'$ . See the inset of Fig. 2 for a plot showing the region in  $(U/t)-(t'/t)$  space where the  $d$ -Mott state is expected.

We now turn to how, in a cold atomic gas, the  $d$ -Mott state could be observed via time-of-flight measurements. First, we suggest a method to generate the  $d$ -Mott state in experiments. To begin, the potential depth of the short period optical lattice is ramped up to a large value  $V_s = 20E_R$  to form a Mott state with one atom per lattice site [6], where  $E_R$  is the photon recoil energy. The potential depth of the long period optical lattice is then ramped up to  $V_l = 17E_R$ . In the Mott state, we have  $t = t' \approx 0$ . To create the  $d$ -Mott state, the potential depth of the short period optical lattice is then ramped down to a small value (for instance,  $V_s = 3E_R$ ) to enhance the tunneling  $t$  inside the plaquettes. The potential barrier between plaquettes is  $V_l + V_s = 20E_R$ , therefore  $t' \approx 0$ . There are now four atoms in each plaquette, which corresponds to the half-filled case discussed above. Nonzero  $t'$  can be obtained by lowering  $V_l$ , and the interaction strength  $U$  can be adjusted in experiments using Feshbach resonance [6]. With this method, various parameter regimes can be reached with different  $U/t$  and  $t'/t$ . For the regime of  $U/t \approx 6$ ,  $t'/\Delta \ll 1$  (i.e.,  $t'/t \ll 0.3$  from Fig. 2), a stable  $d$ -Mott state is obtained.

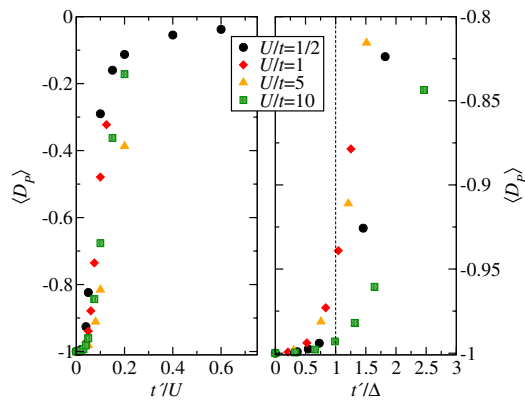


FIG. 3 (color online). Ground state expectation value of the  $d$ -Mott operator,  $\langle D_P \rangle$ , as a function of  $t'/U$  (left) and  $t'/\Delta$  (right) for the eight-site square lattice ladder system for the checkerboard Hubbard model at half filling for various values of  $U/t$ .

We now address the question of the experimental observation of this state.

Interestingly, the phase coherence in each plaquette in the  $d$ -Mott state can be experimentally identified in the time-of-flight (TOF) measurements. The  $d$ -Mott state in a single plaquette can be written as  $|\chi\rangle = \sum_{\alpha} f_{\alpha} |\alpha\rangle$  where  $|\alpha\rangle$  is a basis state such that the action of  $D_P$  on a state rotates it to another basis state and the  $d$ -wave symmetry of the ground state wave function has been incorporated into the eigencoefficients  $f_{\alpha}$ . In the TOF experiment, we can measure the density of the spin-up and spin-down atoms separately. The TOF density distribution for spin-up atoms is

$$\langle n_{\uparrow}(\mathbf{Q}(\mathbf{r})) \rangle \propto \sum_{I, I'} \psi_I^* \psi_{I'} \langle b_I^{\dagger} b_{I'} \rangle \quad (2)$$

where  $\mathbf{Q}(\mathbf{r}) = m\mathbf{r}/\hbar t$  ( $m$  and  $t$  being the atomic mass and time of measurement, respectively),  $I$  is the index of plaquettes,

$$\psi_I \propto e^{-i\mathbf{Q}(\mathbf{r}) \cdot \mathbf{R}_I} \Phi(\mathbf{Q}) \sum_{\alpha} e^{-i\mathbf{Q}(\mathbf{r}) \cdot \sum_{\beta} \beta_{\alpha j} \mathbf{s}_j} f_{\alpha} \quad (3)$$

is the wave function of spin-up atoms in plaquette  $I$  after TOF,  $b_I^{\dagger}$  is the creation operator of the  $d$ -Mott state in the plaquette  $I$ ,  $\mathbf{R}_I$  is the position of the center of plaquette  $I$ ,  $j = 1, 2, 3, 4$  correspond to four lattice sites at each plaquette [see Fig. 4(a)] with  $\mathbf{s}_1 = (-a/2, -a/2)$ ,  $\mathbf{s}_2 = (a/2, -a/2)$ ,  $\mathbf{s}_3 = (a/2, a/2)$ ,  $\mathbf{s}_4 = (-a/2, a/2)$ ,  $a$  is the lattice spacing,  $\beta_{\alpha j}$  is the spin state of atoms at site  $j$  and basis state  $\alpha$ , and  $\Phi(Q)$  is the Fourier transform of the Wannier function at each site. In the  $d$ -Mott state, we have  $\langle b_I^{\dagger} b_{I'} \rangle \propto \delta_{II'}$ , yielding

$$\langle n_{\uparrow}(\mathbf{Q}(\mathbf{r})) \rangle \propto \left| \sum_{\alpha} e^{-i\mathbf{Q}(\mathbf{r}) \cdot \sum_{\beta} \beta_{\alpha j} \mathbf{s}_j} f_{\alpha} \right|^2. \quad (4)$$

In a single plaquette, we find that the  $d$ -Mott ground state can be written as

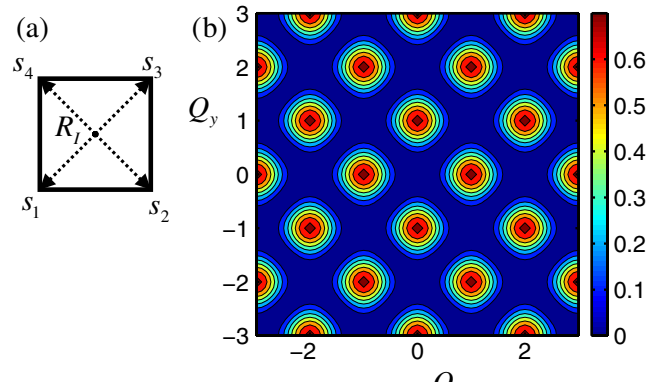


FIG. 4 (color online). (a) A single plaquette  $I$ . (b) Density distribution of  $d$ -Mott state in a time-of-flight experiment. The unit for  $Q_x$  and  $Q_y$  is  $\pi/a$ .  $U/t = 5$ .

$$\begin{aligned}
|\chi_P\rangle = & \sum_{i=1}^4 (-D_P)^{i-1} [(\lambda - \gamma)|1100; 0011\rangle + \gamma|1100; 1100\rangle \\
& - \xi\{|1100; 1010\rangle + |1100; 0101\rangle\}] \\
& + \sum_{i=1}^2 (-D_P)^{i-1} [\xi\{-|1010; 1100\rangle - |1010; 0110\rangle \\
& + |1010; 1001\rangle + |1010; 1010\rangle\}] \\
& + 2(\lambda - \gamma)|1010; 0101\rangle
\end{aligned} \quad (5)$$

where  $\lambda$ ,  $\gamma$ , and  $\xi$  are parameters determined by  $(U, t, t')$  and satisfy normalization  $[16\xi^2 + 12(\lambda - \gamma)^2 + 4\gamma^2 = 1]$ . When  $U \rightarrow \infty$ ,  $\lambda \rightarrow \sqrt{3}/6$ ,  $\xi \rightarrow 0$ ,  $\gamma \rightarrow 0$  and the state becomes

$$\begin{aligned}
|\chi_P\rangle \rightarrow & \frac{\sqrt{3}}{6}(|1100; 0011\rangle - |0110; 1001\rangle + |0011; 1100\rangle \\
& - |1001; 0110\rangle) + \frac{\sqrt{3}}{3}(|1010; 0101\rangle - |0101; 1010\rangle)
\end{aligned} \quad (6)$$

which has no double occupancy. Under the operation of  $D_P$  onto  $|\chi_P\rangle$  [either Eq. (5) or Eq. (6)], it is seen that an eigenvalue of  $-1$  is obtained. Using the wave function [Eq. (5)] and Eq. (4), we find

$$\langle n_i(\mathbf{Q}(\mathbf{r})) \rangle \propto 4\lambda^2 |\cos(Q_x a) - \cos(Q_y a)|^2. \quad (7)$$

Note that the ground state of  $H$  (Eq. (1) with finite  $t'$ ) is approximately the  $d$ -Mott state when  $\langle D_P \rangle \approx -1$  and, hence, it is approximately described by a product state of single plaquette ground states [Eq. (5)] with a TOF density distribution given by Eq. (7).

In Fig. 4(b), we plot the density distribution for the  $d$ -Mott state in TOF measurements with the image showing interference peaks at  $Q_x + Q_y = N\pi/a$ , where  $N$  is an odd integer and  $Q_x$  and  $Q_y$  are multiples of  $\pi/a$ . We want to emphasize that these peaks disappear in the TOF for a pure Mott state where one should observe a flat background, and this would be a way to contrast the present state from a regular Mott insulator. Further, the behavior of  $\langle D_P \rangle$  as a function of  $t'$  (Fig. 3) is exactly indicative of the “ $d$ -Mott”-ness of the ground state of  $H$  with a TOF signature shown in Fig. 4(b). Therefore, monitoring the TOF interference peaks while varying  $U/t$  and  $t'/t$  would be an effective way to observe the  $d$ -Mott state.

In Fig. 5, we plot the coefficient  $4\lambda^2$  with respect to the on-site energy  $U$  and find that the signal strength increases reaching  $4/3$  for  $U \rightarrow \infty$ . However, the  $d$ -Mott state signal may not be observable for large  $U$  because the gap  $\Delta$  is small at large  $U$  (see Fig. 2), where a small interplaquette tunneling  $t'$  may mix the  $d$ -Mott state with other states [see Fig. 3(b)], destroying the order and removing the interference signal. This is expected because for  $U \rightarrow \infty$ , the system is in a pure Mott state where no interference peaks are expected. Another possible roadblock in the path of observing the interference pattern is that the temperature of the system must also be below  $\Delta$  so that thermal fluctua-

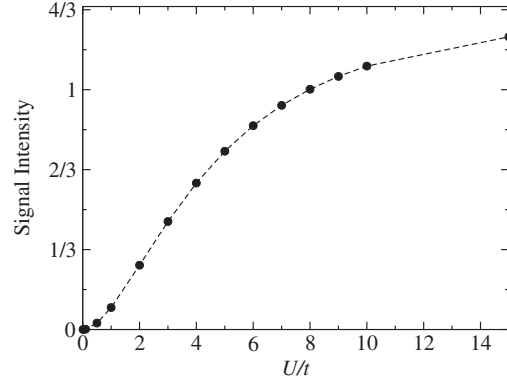


FIG. 5. Signal intensity  $4\lambda^2$  versus  $U/t$ .

tions do not destroy the  $d$ -Mott order. But using  $U/t \approx 5-6$  and keeping  $k_B T \ll \Delta$  should lead to the experimental observation of the  $d$ -Mott state.

To conclude, we have described a scenario where a new state of matter, the  $d$ -Mott insulator, could be observed in a fermionic optical lattice via TOF measurements. Furthermore, we have provided semiquantitative parameter values where the state should most likely be seen ( $U/t \approx 6$  and  $t'/t < 0.3$ ). This could also serve as a rigorous benchmark in further experimental studies toward the realization of the general two-dimensional square lattice Hubbard model in relation to its utility in the study of high- $T_C$  cuprate superconductors. We believe that the direct TOF observation of the hitherto-unobserved  $d$ -Mott quantum insulator in a fermionic optical lattice would go a long way in establishing cold atomic gases as a useful optical lattice emulator of novel strongly correlated phases.

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