Mott-Insulator to Superconductor Transition in a Two-Dimensional Superlattice

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We use quantum Monte Carlo and exact diagonalization calculations to study the Mott-insulator to superconductor quantum phase transition in a two-dimensional fermionic Hubbard model with attractive interactions in the presence of a superlattice potential. The model introduced offers unique possibilities to study such transitions in optical lattice experiments. We show that, in regimes with moderate to strong interactions, the transition belongs to the $3D-XY$ universality class. We also explore the character of the lowest energy charge excitations in the insulating and superconducting phases and show that they can be fermionic or bosonic depending on the parameters chosen.

PACS numbers: 71.10.Fd, 02.70.Uu

Introduction. The traditional microscopic approach to understanding superconductivity scrutinizes the pairing instability of a “parent” normal state \[i\]. If this normal state is not a conventional state of weakly interacting electrons (i.e., a Fermi liquid or a band-insulator), then the emerging superconductivity is not ordinary either. Many superconductors fall in this category, including organic, heavy-fermion, and all high-temperature ones (cuprates and iron-based). Non-trivial electron correlations behind superconductivity are most famously seen in the “pseudogap” state of cuprates, and are very difficult to understand from experimental observations \[2–9\]. This is where ultracold-atom systems, which are highly tunable, are expected to help. However, the temperatures required to realize the $d$-wave pairing of cuprates remain prohibitively low for current ultracold atom experiments \[10\]. Even obtaining long-range antiferromagnetic correlations in a three-dimensional Mott insulator remains a challenge \[11,13\].

With these challenges in mind, it is desirable to design $s$-wave paired states that would make the “pseudogap” physics accessible to current experiments with ultracold fermions in optical lattices. In this letter, we study a zero temperature Mott insulator of bound Cooper pairs, which gives rise to the $s$-wave analogue of a pseudogap state, as well as to a superconductor upon changing lattice parameters. We consider a Fermi-Hubbard model in the square lattice and in the presence of a superlattice potential. The Hamiltonian reads

\begin{align*}
\hat{H} = & -t \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.}) - t' \sum_{\langle \langle i,j \rangle \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{H.c.}) \\
+ & U \sum_i \left( \hat{n}_{i\uparrow} - \frac{1}{2} \right) \left( \hat{n}_{i\downarrow} - \frac{1}{2} \right) + \Delta \sum_{i,\sigma} (-1)^{\langle i \rangle \langle i \rangle} \hat{n}_{i\sigma},
\end{align*}

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) are the fermionic creation (annihilation) operators at site $i$, with (pseudo-)spin $\sigma = \uparrow, \downarrow$, and $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$ are the corresponding site occupation operators. The nearest and next-nearest hopping amplitudes are denoted by $t$ and $t'$ \[\langle i \rangle \langle j \rangle\] and \[\langle \langle i \rangle \rangle \langle \langle j \rangle \rangle\] indicate sums over nearest and next-nearest neighbor sites $i$ and $j$, respectively, the strength of the on-site attractive interaction by $U < 0$, and of the staggered potential by $\Delta$.

In experiments, attractive interactions between atoms can be generated using Feshbach resonances \[14\], optical superlattices can be created using arrays of laser beams \[15,17\], and periodically modulated optical lattices allow to control the relative amplitudes and phases between nearest and next-nearest neighbor hopping parameters \[18,19\]. A recent experimental realization of the Haldane model exemplifies these capabilities \[20\].

To show what makes the model in Eq. (1) special to study Mott-insulator to superconductor phase transitions in optical lattice experiments and theoretically, we analyze it in two limits. First, let us consider the non-interacting limit \((U = 0)\). The Hamiltonian can be diagonalized in $k$-space, which unveils two bands, $E(k) = -4t' \cos k_x k_y \pm \sqrt{\epsilon_{k_x}^2 + \Delta^2}$, where the reduced Brillouin zone is given by $|k_x| + |k_y| \leq \pi$ and $|k_x - k_y| \leq \pi$, and $\epsilon_{k} = -2t \cos (k_x) + \cos (k_y)$ is the dispersion relation in the presence only of nearest neighbors hopping. For $t' < t/\sqrt{2}$, an indirect gap opens for $\Delta_c = 2t'$ [between $(\pm \pi, 0)$] in the lower band and $(\pm \pi/2, \pm \pi/2)$ in the upper band. For $t' > t/\sqrt{2}$, an indirect gap opens for $\Delta_c = 4t' - t^2/t' [between (\pm \pi, 0)$] in the lower band and $(0, 0)$ in the upper band]. $\Delta_c$ is then the critical value of $\Delta$ for the formation of a band insulator at half filling, i.e., a finite value of $t'$ stabilizes a metallic state for small, but nonzero, values of $\Delta$.

The second important limit is the one in which $U/t \neq 0$ but $t' = 0$. Recalling that the attractive Hubbard Hamiltonian can be mapped onto a repulsive one by the down-spin particle-hole transformation \[21\], $\hat{c}_{i\sigma}^\dagger \leftrightarrow (-1)^{i_x + i_y} \hat{c}_{i\sigma}^\dagger$, the staggered potential transforms as $\Delta \sum_{i\sigma} (-1)^{\langle i \rangle \langle i \rangle} \hat{n}_{i\sigma} \rightarrow h \sum_{i\sigma} (-1)^{\langle i \rangle \langle i \rangle} \hat{S}_{i\sigma}^z$, with $\hat{S}_{i\sigma}^z = (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})/2$ and $h = 2\Delta$. Therefore, at half-filling, the staggered potential in the attractive model is
equivalent to a staggered $z$-magnetic field in the repulsive one. For $h = 0$, the ground state of the repulsive Hubbard model is an $SU(2)$ symmetric Mott insulator that exhibits long-range antiferromagnetic correlations. Those translate onto long-range $s$-wave superconducting order and charge density-wave order in the attractive model (i.e., a supersolid) [21]. An infinitesimal $h$ breaks $SU(2)$ symmetry and the ground state of the repulsive model becomes an $S^z$ antiferromagnet, which translates onto a (charge density-wave) Mott insulator in the attractive case, i.e., superconductivity is destroyed for any nonzero value of $\Delta$. For large values of $h$, this insulator can be understood to be the result of pinning the pairs to the sites with energies $-\Delta$, which precludes transport.

Hence, if one takes the noninteracting limit as the starting point, adding weak attractive interactions generates superconductivity in the metallic phase, i.e., when $t' \neq 0$, superconductivity can be stabilized for nonzero values of $\Delta$. However, the bandgap opened when $\Delta > \Delta_c$ can destroy this superconductor in favor of a Mott-insulator. Such a transition is the focus of this work. It can be driven in real time in an optical lattice experiment by modifying lattice parameters. This is to be contrasted to the Mott-insulator to superconductor transition in the cuprates, which requires changing doping, i.e., in an optical lattice experiment one would need to change the filling in real time to drive such a transition.

We study Hamiltonian (1) in $L \times L$ lattices using two unbiased computational approaches: zero-temperature (projector) determinantal quantum Monte Carlo (PDQMC) [22][23] and Lanczos exact diagonalization (ED). We focus on half-filled systems ($n = \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle = 1.0$, $\langle n_{i\uparrow} \rangle = \langle n_{i\downarrow} \rangle$), except when analyzing the nature of the charge excitations. The projector parameter in the PDQMC calculations was set to $\Theta t = 40$, ensuring that we obtain ground state properties for lattices with up to 256 sites, while the imaginary time discretization step was taken to be $\delta \tau = 0.1$. In the ED calculations, we used translational symmetries, which allowed us to solve lattices with up to 16 sites. $t = 1$ sets the energy scale in all results reported in what follows.

Results. Figure 1 depicts the phase diagram for Eq. (1), obtained using ED [Fig. 1(a)] and PDQMC [Fig. 1(b)], as given by the $\Delta_c$ necessary to drive the superconductor to Mott-insulator transition as a function of $|U|$ and $t'$. Important features visible in Fig. 1 are, (i) $\Delta_c$ decreases with increasing $|U|$, and, (ii) as expected from the discussion in the noninteracting limit, $\Delta_c$ increases with increasing $t'$. The first trend can be understood as both the attractive interaction and the staggered potential favor local pair formation and, consequently, reduce long-range order when $\Delta \neq 0$ and $|U|$ is increased. The second trend follows from the fact that the delocalization promoted by $t'$ competes with the pinning induced by $\Delta$ and $U$, and enhances superconductivity.

In the ED calculations, in order to determine $\Delta_c$ for the superconductor to Mott-insulator transition at fixed $U$ and $t'$, we use the ground-state fidelity metric [24][30]

$$g(\Delta) = \frac{2}{\langle \delta \Delta \rangle^2} \left( 1 - |\langle \Psi_0(\Delta) | \Psi_0(\Delta + \delta \Delta) \rangle| \right),$$

where $|\Psi_0(\Delta)\rangle$ is the ground-state wavefunction of the Hamiltonian for a given staggered on-site energy $\Delta$ and $\delta \Delta$ is chosen to be small enough that the results for $g(\Delta)$ are independent of its value. $g(\Delta)$ is expected to exhibit a diverging (with increasing system size) maximum as one crosses a second order phase transition [24][30].

Figures 2(a)–2(c) depict the fidelity metric for different values of the onsite interaction ($U = -2, -4$ and $-6$, respectively) and for four values of $t'$ ($t' = 0.0, 0.2, 0.4$ and $0.6$). For $t' = 0$ and all values of $U$, one can see that there is a single peak in $g$ for $\Delta \simeq 0$. This peak signals the supersolid to Mott-insulator transition previously discussed for the limit $U \neq 0$ but $t' = 0$. The signature of such a transition can still be seen for $t' \neq 0$ in the form of a peak at $\Delta \simeq 0$ with a height that decreases with increasing $t'$ (notice the log scale in the $y$-axes). A second peak then emerges for $t' \neq 0$ signaling the superconductor to Mott-insulator transition with increasing $\Delta$. We take the position of the maximum of this peak as the value of $\Delta_c$ predicted by ED. The compilation of these peak positions provides the phase diagram reported in Fig. 1(a). Notice that, with increasing $|U|$, the positions of the peaks for a given value of $t'$ move towards smaller values of $\Delta$. They also become broader and at some point merge with the one at $\Delta \simeq 0$. At that point, we cannot determine $\Delta_c$ using ED. This is why the phase diagram in Fig. 1(a) is missing points for large $|U|$, small $t'$, values.

The PDQMC calculations have the advantage that they allow us to study much larger lattice sizes and, after a proper finite-size scaling analysis, determine $\Delta_c$ in the thermodynamic limit. We take the pair structure factor $P = \sum_{i,j} \langle \tilde{c}_{i\uparrow} \tilde{c}_{j\downarrow} \rangle$, with $\tilde{c}_{i\sigma} = c_{i\sigma} e^{i\xi}$, to be the
order parameter to locate the superconductor to Mott-insulator transition (other observables give consistent results, see Ref. [31]). The limit $|U|/t \gg 1$, for $t' = 0$, provides guidance on the nature of the superconductor to Mott-insulator transition for strong attractive interactions. Second-order perturbation theory in $t/|U|$ reveals that Eq. (1) becomes equivalent to a Hamiltonian for hard-core bosons with site creation (annihilation) operator $\hat{b}^\dagger_i = \hat{P}^\dagger_i (\hat{b}_i = \hat{P}_i)$ [21, 32] in a superlattice. The phase diagram for the latter model was studied in Refs. [33, 34] in two (2D) and three (3D) dimensions. At half-filling, this model exhibits a superfluid to Mott-insulator transition with increasing $\Delta$ that belongs to the $(d+1)$-XY universality class [33, 34], like the integer filling Mott transition in the Bose-Hubbard model [35]. The addition of $t'$ to the hard-core boson model does not break its particle-hole symmetry. Hence, it does not qualitatively change the phase diagram in Refs. [33, 34].

Remarkably, at half-filling, the pair structure factor can also be written as $P = \sum_{i,j} (\hat{P}^\dagger_i \hat{P}_j)$, i.e., it maps onto the zero momentum mode occupation in the hard-core boson model, $m_{k=0} = \sum_{i,j} (\hat{b}_i^\dagger \hat{b}_j)$. In the insulating phase of the latter quantum system in 2D one expects $\langle \hat{b}_i^\dagger \hat{b}_{i+r} \rangle \propto e^{-r/\xi}$ at long distances, as in the corresponding disordered 3D classical phase, where $\eta = 0.0381 \pm 0.0002$ [33] is the anomalous scaling dimension and $\xi$ the correlations length. Near the transition, $m_{k=0}$ diverges with $\xi$ as $m_{k=0} \sim \xi^{1-\eta}$ [37, 38] and the fraction $f_0$ of pairs that condense in a finite system ($\xi \to L$) vanishes as $f_0 \sim L^{-(1+\eta)}$ [37, 38]. Hence, $f_0$ scales as $f_0 L^{1+\eta} = F(|\Delta - \Delta_c| L^{1/\nu})$ [38], with $\nu = 0.6717 \pm 0.0001$ [36]. Turning back to fermions, we can write

$$\langle P/N_{\text{pairs}} \rangle L^{1+\eta} = F(|\Delta - \Delta_c| L^{1/\nu}),$$

where the number of pairs is $N_{\text{pairs}} = L^2/2$.

Figure 2 shows the scaled pair-structure factor vs $\Delta$ for two values of $U$ and two values of $t'$. In all cases the curves cross at a single point ($\Delta_c$), as expected from the scaling ansatz [3]. That point moves toward larger values of $\Delta_c$ from Fig. 2(a) to Fig. 2(b), as $t'$ is increased at constant $U$, and moves toward smaller values of $\Delta_c$ from Fig. 2(b) to Fig. 2(c), as $|U|$ is increased at constant $t'$. The insets show that, close to the crossing points, the data exhibits an almost perfect collapse according to the scaling ansatz [3]. They confirm that, for those values of $U$, the superconductor to Mott-insulator transition in our fermionic model belongs to the 3D XY universality class. This despite the fact that the results are for a regime in which $|U|$ is of the order of 1/2 the bandwidth of the non-interacting system with $\Delta = t' = 0$ and, as such, strong coupling perturbation theory is not appropriate to describe the system. A compilation of crossing points as those in Fig. 2 allowed us to generate the phase diagram...
The observed 3D-XY universality class of the superconductor–Mott-insulator transition indicates that the lowest-energy charge excitations have bosonic character in both the superconducting and insulating phases near the transition. However, the lowest-energy excitations of our model must be fermionic deep in the insulating phase. The insulating region with bosonic low-energy excitations is the $s$-wave equivalent of the pseudogap state (a crossover regime rather than a thermodynamic phase). In what follows, we explore when the lowest charge excitations change from bosonic to fermionic. In Fig. 3 we show the ground-state energy at half-filling as well as the energies of the lowest excited states with two extra fermions ($S^z = 0$, lowest energy bosonic excitation) and an extra fermion ($S^z = 1/2$, lowest energy fermionic excitation) as a function of $\Delta$ for two values of $U$ and two values of $t'$.

Figures 4(a) and 4(b) show that, for the values of $\Delta$ at which the superconductor to Mott-insulator transition occurs for $U = -6$, the lowest energy excitations in both phases are bosonic. However, there is a value of $\Delta > \Delta_c$ for which the lowest charge excitation (within the Mott insulating phase) changes from bosonic to fermionic. That value of $\Delta$ decreases as $t'$ increases [Fig. 4(a) vs Fig. 4(b)] and as $U$ decreases [left panels vs right panels in Fig. 4]. For $U = -4$ [Figs. 4(c) and 4(d)], the ED calculation predicts the transition from bosonic to fermionic excitations to occur in the Mott phase for $t' = 0$ and in the superconducting phase for $t' = 0.2$. The latter is attributed to finite size effects as it contradicts the expectation from the PDQMC results. Also, in the weak coupling limit, field-theory arguments anticipate that the transition should be in the XY universality class $[39, 40]$. These results are nontrivial, even though any attractive short-range potential gives rise to bound states (Cooper “molecules”) in 2D, because if interactions are not strong enough those “molecules” need not be small in comparison to the interparticle separation, i.e., bound-state condensation need not occur.

**Summary.** We have introduced and studied a 2D model that undergoes a superconductor to insulator transition. We determined its phase diagram using ED and PDQMC calculations, and showed that, in the parameter regime accessible to PDQMC, the transition belongs to the 3D-XY universality class. Our results echo the well-known XY transition of the bosonic Hubbard model, but in a fermionic system. We explored the nature of the lowest energy charge excitations and showed that they change from bosonic to fermionic in the insulating phase.

Our numerical demonstration of “pseudogap” physics in a realizable model aims to enable a new route for the experimental exploration of high-temperature superconductivity using ultracold atoms. While there are clearly many microscopic differences between our model and real superconductors, there are also several universal similarities that can be exploited. Most notably, the dynamics of our system shares a lot in common with charge and vortex dynamics near the superconducting transition in layered or quasi-2D superconductors.

**Acknowledgments** This work was supported by the National Science Foundation Grants No. PHY13-18303 (R.M., M.R.) and PHY-1205571 (P.N.), and by CNPq (R.M.). The computations were performed in the Institute for CyberScience at Penn State, the Center for High-Performance Computing at the University of Southern California, and CENAPAD-SP.

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Supplementary Materials:
Mott-Insulator to Superconductor Transition in a Two-Dimensional Superlattice

EXACT DIAGONALIZATION (ED)

In the presence of the superlattice (staggered) potential, the sublattices forming the bipartite square lattice possess different onsite energies and, consequently, the site occupation is different in the two sublattices. Figures 5(a)–5(d) display the site occupation in each sublattice as a function of $\Delta$ for $U = -2$ (as in the main text, $t$ sets our energy scale) and several values of $t'$. As expected, as $\Delta$ increases, the difference between the site occupation in the sublattices increases. Remarkably, there is a sharp increase in this difference that occurs exactly at the value of $\Delta$ for which the fidelity metric predicts the superconductor to Mott-insulator transition. This sharp increase leads to a sharp peak in the derivative of the site occupation with respect to $\Delta$, see Figs. 5(e)–5(h), which resembles the peak seen in the fidelity metric.

Another observable that exhibits clear signatures of the superconductor to Mott-insulator transition is the binding energy

$$E_b = 2E_0(n+1) - E_0(n+2) - E_0(n),$$

where $E_0(n)$ correspond to the ground state energy of a system with $n$ fermions.

Figure 6 shows the binding energy vs $\Delta$ for different values of $U$ and $t'$. The trend is similar in all of them:

for small values of $\Delta$, before the superconductor to Mott-insulator transition for nonzero $t'$ takes place, the energy associated with the pairs decreases, and then a dip occurs exactly at the transition point as detected by the fidelity metric. For larger values of $\Delta$, in the Mott insulating phase, the binding energy steadily increases with increasing $\Delta$.

Summarizing, the ED results for various observables studied indicate the occurrence of the superconductor to Mott-insulator transition at exactly the same value of $\Delta$ as the fidelity metric. Hence, the results reported in the main text are robust against the selection of the observable.

PROJECTOR DETERMINANTAL QUANTUM MONTE CARLO (PDQMC)

Similar robustness against the selection of the observable used to characterize the transition is seen in the PDQMC calculations of much larger lattice sizes than those amenable to exact diagonalization. An observable of much interest in experiments with ultracold fermions in optical lattices is the double occupancy. It was used, e.g., in Ref. [41] to detect the Mott insulating phase when increasing the onsite repulsion between fermions. In Fig. 7 we plot the double occupancy in the two sublattices vs $\Delta$ for $U = -4$ and different values of $t'$ in a $14 \times 14$ lattice. A kink can be seen in the behavior of this
observable around (slightly after) the critical value of $\Delta$ obtained in the finite size scaling of the pair structure factor (see the main text).

Another local quantity that exhibits a clear signature of the superconductor to Mott-insulator transition is the kinetic energy associated with next-nearest neighbor hopping, i.e., $k_{NNN} = -(t'/N) \sum_{\langle i,j \rangle,\sigma} \langle \hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \rangle$, where $N = L \times L$. As shown in Figs. 8(a)–8(c), the absolute value of $k_{NNN}$ decreases with increasing $\Delta$. This observable also exhibits a kink right after $\Delta_c$ as predicted by the scaling analysis in the main text. The derivatives of $k_{NNN}$ with respect to $\Delta$, shown in Figs. 8(d)–8(f), exhibit clear peaks about $\Delta_c$ with maxima right before the value of $\Delta_c$ reported in the main text.

These observables provide evidence of the robustness of the value of $\Delta_c$ reported in the main text against the selection of the observable in our PDQMC calculations.