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Doped singlet-pair crystal in the Hubbard model on the checkerboard lattice

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In the limit of large nearest-neighbor and on-site Coulomb repulsions, the Hubbard model on the planar pyrochlore lattice maps, near quarter filling, onto a doped, quantum, fully packed loop model. The phase diagram exhibits at quarter filling a quantum state of matter, the resonating singlet-pair crystal, an insulating phase breaking lattice symmetry. Properties of a few doped holes or electrons are investigated. In contrast to the doped quantum antiferromagnet, phase separation is restricted to very small hopping, leaving an extended "window" for superconducting pairing. However, the latter is more fragile for large hopping than in the case of the antiferromagnet. The existence of a fermionic supersolid is discussed.

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Correlated fermions and bosons on frustrated lattices exhibit fascinating properties. For example, on the triangular lattice, hard-core bosons with *nearest-neighbor* (NN) repulsion can realize a supersolid phase exhibiting both charge order and superfluidity.[1] In the light of recent scanning tunneling microscopy experiments suggesting the coexistence of superconductivity and charge order,[2] it is interesting to ask whether a fermionic analog of a supersolid could be realized by doping a Mott insulator whose ground state spontaneously breaks lattice symmetries?

In this Rapid Communication, we study correlated fermions on the checkerboard lattice (sketched on Fig. 1), a two-dimensional array of corner-sharing tetrahedra. This is a two-dimensional analog of the pyrochlore lattice found in numerous spinel and pyrochlore materials.[3] For a filling of exactly half an electron per site, extremely strong on-site and NN repulsion selects a macroscopically degenerate manifold of low-energy configurations satisfying the so-called "ice rules" constraint, i.e., having exactly two particles per tetrahedron. These can be mapped onto the configuration space of a six-vertex model.[4] By associating each particle with a dimer joining the centers of the two corner-sharing tetrahedra, an alternative *fully packed loop representation* can be obtained. Although the constrained quantum dynamics of bosons[5] and spinless fermions[6] differ, the phase diagrams of these models contain a rich variety of crystalline phases breaking lattice translations and/or rotations. In addition, fractionalization of a doped charge e into two $e/2$ components can also appear under some conditions.[6–8]

Here, we consider the realistic case of *spinful* fermions (electrons), whose spin degrees of freedom play a central role. We show that the quarter-filled ground state (GS) is an insulating crystalline quantum state involving resonant spin-singlet electron pairs. We then argue, on the basis of numerical calculations, that pairing can emerge under light doping. Such a superconductor is expected to break lattice symmetries in a similar way to the supersolid of Ref. 1 (although with no charge ordering). One of the most exciting applications of these ideas is to assemblies of cold atoms in optical lattices, where models of the form we propose can, in principle, be realized by the appropriate tuning of atomic interactions.[9]

The model. Our starting point is a (fermionic) Hubbard model extended with nearest-neighbor ($\langle ij\rangle$ in the sum) repulsion V on the checkerboard lattice:

$$\mathcal{H} = -t\sum_{\langle ij\rangle}(f^{\dagger}_{i\sigma}f_{j\sigma} + \text{H.c.}) + V\sum_{\langle ij\rangle} n_i n_j + U\sum_i n_{i\uparrow}n_{i\downarrow} \quad (1)$$

using standard notation. We are interested in the limit where the on-site repulsion U is very large, forbidding double occupancy. Furthermore, we consider the limit $V \gg t$, in which case, for quarter filling $\left(\langle n_i\rangle = \frac{1}{2}\right)$, the ground state is an insulator. Expanding about this state, we obtain, to leading order, the effective Hamiltonian

$$\mathcal{H}_{\square} = -t_2\sum_{\square}(f^{\dagger}_{i\uparrow}f^{\dagger}_{j\downarrow} - f^{\dagger}_{i\downarrow}f^{\dagger}_{j\uparrow})(f_{k\downarrow}f_{l\uparrow} - f_{k\uparrow}f_{l\downarrow}) + \text{H.c.}, \quad (2)$$

where $t_2 = 2t^2/V$ and the summation runs over the "empty squares" of the checkerboard lattice, with the sites of a given square counted $ikjl$. $\mathcal{H}_{\square}$ acts on two electrons, forming a singlet on the diagonal kl, transferring that singlet to the (empty) perpendicular diagonal ij.

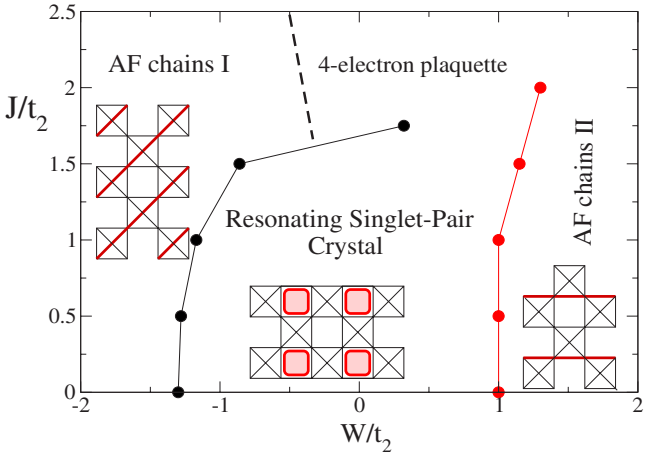

FIG. 1. (Color online) Proposed phase diagram as a function of W and J. See text for a description of the relevant phases.

We also introduce a diagonal term which counts the squares where $\mathcal{H}_{\square}$ can act,

$$\mathcal{H}_W = W\sum_{\square}\left(\frac{1}{2} - 2\mathbf{S}_i\cdot\mathbf{S}_j\right)n_i n_j(1-n_l)(1-n_k). \qquad (3)$$

For $W \equiv t_2$, the Hamiltonian $\mathcal{H}_{\square}+\mathcal{H}_W$ becomes a sum of projectors, and we recover the physics of the quantum dimer model[10] at the Rokhsar-Kivelson point: the GS can be written exactly as an equal-weight superposition of all zero-energy configurations.[10] This nontrivial property also holds in the presence of static holes ($t=0$).

Finally, we also include the two-site spin exchange

$$H_J = -J\sum_{\langle ij\rangle}\left(\frac{1}{4} - \mathbf{S}_i\cdot\mathbf{S}_j\right)n_i n_j, \qquad (4)$$

where, for $U \gg V \gg t$, the exchange constant J is given by the ratio $J/t_2 \simeq 2V/U + 4t/V$. For the undoped system, J/t_2 is therefore the only parameter (whose physical absolute value should typically be smaller than 1), the connection with the Hubbard model being realized for $W=0$. Here we consider only antiferromagnetic (AF) coupling, $J>0$.

Away from quarter filling, when N_h holes (or electrons) are introduced, simple counting shows that exactly $2N_h$ tetrahedra (named hereafter "half-hole tetrahedra") should contain a single, shared electron (or three shared electrons for electron doping). All other tetrahedra contain exactly two shared electrons, as before; violation of this constraint would lead to an energy increase of order V. The single hopping term t then becomes effective by moving around the locations of these "fractional charges."[7] We have performed extensive Lanczos exact diagonalization (ED) on a periodic (45° tilted) square cluster of $N=32$ sites in the insulator and for a small number of doped holes or electrons.[11]

Phase diagram at quarter filling. For $J=0$, by analogy with Ref. 5 and from simple analytic arguments, we expect to have, as a function of W, (i) for large negative W, parallel spin chains; (ii) for intermediate $|W|$ values, a resonating singlet-pair crystal (RSPC); (iii) for $W=t_2$, a liquid-like "RK" point; (iv) for $W>t_2$, a manifold of isolated states (which include all ferromagnetic states), all having $E=0$. This picture is indeed supported by our ED calculations [see Fig. 2(a)], where the characterization of the various phases (see Fig. 1) can be obtained from the analysis of the low-energy spectrum. In the two fold-degenerate RSPC, electron pairs resonate in every second void plaquette, breaking translational symmetry. This is seen numerically in the collapse of a $\mathbf{k}=(\pi,\pi)$ A_1 symmetry[12] singlet excited state onto the GS [Fig. 2(a)]. For sufficiently negative W, the electrons order along diagonal chains to optimize the Heisenberg exchange along the diagonals of the empty squares, hence breaking rotation symmetry. This is seen in the ED spectrum as the quasidegeneracy of the $(\mathbf{k}=\mathbf{0},B_1)$ singlet and the GS. For $W>1$, isolated states where the plaquette resonance is ineffective (including the horizontal chains shown), are favored.

Note that a perturbative expansion about isolated void plaquettes[13] gives a very accurate estimate of the RSPC GS energy (for $J=0$). Already, in first order—$E^{(1)}=N(\frac{33}{64}W-\frac{1}{2}t_2)$, as shown in Fig. 2—the agreement is excellent. A comparison to a similar expansion from disconnected diagonal chains gives an estimate of the boundary between the two phases in full agreement with the numerics, although it suggests that the actual critical value shifts to more negative W in the thermodynamic limit. One should point out that (i) in contrast to the bosonic case,[5] the range of stability of the plaquette phase is much broader on the W axis and (ii) as shown in Fig. 2(b) and Fig. 1, the RSPC is also very stable when the exchange J is included. Only above $J/t_2 \sim 1.5$ is a new phase of four-electron plaquettes oriented along the $(1,\pm 1)$ directions stabilized by a gain of exchange energy (small Heisenberg loops have higher quantum fluctuations).[14] Lastly, we stress that our RSPC at $J/t_2 < 1.5$ differs from the bond order wave realized for $t>0$ at intermediate V/t ratio (for which charge fluctuations still occur),[15] which shows two kinds of *criss-crossed* plaquettes. Indeed, although both phases exhibit a doubling of the unit cell (neither with charge ordering), they differ in the type of resonating plaquette.

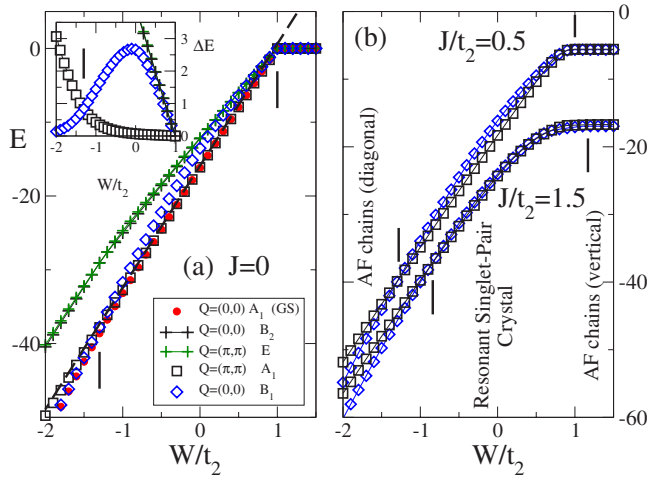

FIG. 2. (Color online) Energies of the 1/4 filled GS and singlet excited states characterized by different quantum numbers (as shown) vs W for $J=0$ (a). Inset: energy differences with respect to GS. (b) Same data for excited states only, and finite values of J. Phase transitions (shown by vertical bars) are signaled by the crossing between excited states (left) and by a W-independent energy (right). The dashed line in (a) shows the $E^{(1)}$ perturbation result (see text).

Finite doping. In investigating the effect of doping, we restrict to ourselves $W=0$ and consider only values of J for which the RSPC is realized at zero doping.

A single doped hole (or electron), as discussed above, is in fact split into two mobile half-hole tetrahedra carrying one electron only (and effective charge $e/2$).[6,7] For reasons similar to those given in Ref. 6, one expects a confining potential so that a small quasiparticle weight survives (in fact, in the $t=0$ limit, the two half-hole tetrahedra even share a common site). In order to estimate the coherent bandwidth, we have computed by ED the GS energy of a single hole for various inequivalent $\mathbf{k}$ momenta,[16] and results are reported in Fig. 3. For large t (compared to t_2 or J), the bandwidth is reduced by, roughly, a factor $t_2/|t|$ (or $J/|t|$) for $t>0$, or even more for $t<0$, and the hole becomes quite massive. This is very reminiscent of the behavior of a single hole doped in a quan-

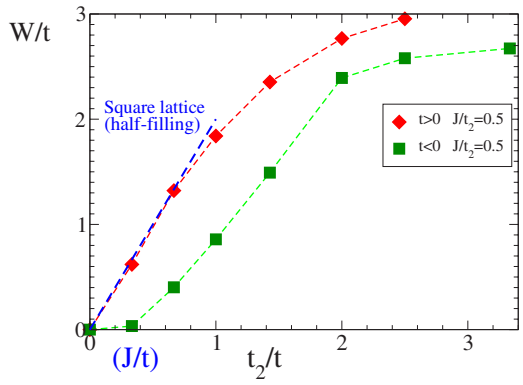

FIG. 3. (Color online) Single hole bandwidth (in units of $|t|$) as a function of $t_2/|t|$ for a fixed (physical) ratio of J/t_2. For comparison, the same quantity for the quantum AF on the square lattice is indicated, as a function of J/t, by a dashed (blue) line.

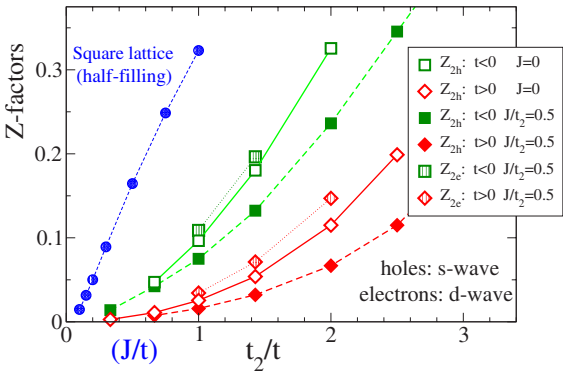

FIG. 4. (Color online) Two-hole Z factor Z_{2h} versus $t_2/|t|$ for $J=0$ and $J/t_2=0.5$. The case of two doped electrons is also shown (Z_{2e}) as hashed symbols (for $J=0.5$). For comparison, the same quantity is shown as circles (blue online) for two holes doped into the quantum AF on the square lattice vs J/t [data for a 26-site cluster (Ref. 19)].

tum antiferromagnet (shown also in Fig. 3 for comparison), where the hole leaves behind a path of flipped spins which can be healed over a short time scale proportional to $1/J$ by spin fluctuations.[17] We believe a similar path exists here also behind the moving hole, along which the plaquette order is perturbed.

As the effective Hamiltonian lowers the energy of singlet pairs, it is natural to study the emergence of pairing interaction. For $t=0$ we found that two holes are next to each other or, more precisely, that all four half-hole tetrahedra are fully packed around a single void plaquette, in order to minimize plaquette resonance and bond exchange energies. The two-hole GS for $t=0$ can be very well approximated by $|\Psi_{2h}^0\rangle \simeq \Delta_s^\dagger |\Psi_0\rangle$ where $\Delta_s^\dagger$ removes two electrons along the diagonals of a void plaquette with s-wave orbital symmetry. For finite t, it is therefore convenient to define the overlap squared, $Z_{2h}=|\langle\Psi_{2h}|\Psi_{2h}^0\rangle|^2$, to get an accurate estimate of the so-called two-hole Z factor $|\langle\Psi_{2h}|\Delta_s^\dagger|\Psi_0\rangle|^2$. Note that $|\Psi_{2h}^0\rangle$ is now defined as a Bloch state with the same momentum as the two-hole GS $|\Psi_{2h}\rangle$ [typically $\mathbf{k}=(0,0)$], i.e., as a linear superposition of all local (degenerate) hole pair states. On increasing $|t|$, Z_{2h} should remain finite as long as the holes stay bound. Figure 4 shows that Z_{2h} is more rapidly suppressed than for two holes in an AF (shown also in Fig. 4 for comparison),[19] suggesting that the hole pair is more fragile here for large $|t|/t_2$ and $|t|/J$ values. A very similar behavior is also found for two doped electrons (see Fig. 4), although the related bound state now has d-wave symmetry.[18]

To get a more direct insight into the tendency of a hole pair to break up at large $|t|/t_2$, we have computed the pair binding energy $\Delta_{2h}=E_{2h}+E_{0h}-2E_{1h}$ shown in Fig. 5, where E_{mh} is the GS energy of the system with $N_h=m$ holes. From its definition, negative Δ_{2h} suggests the binding of the holes, as previously seen in a doped Heisenberg AF on a square lattice [in blue (gray)]—even for rather large hole kinetic energy. On the contrary, the data for the 1/4 filled checkerboard lattice do not provide evidence of binding when $t/t_2>1$. Note, however, that Δ_{2h} is subject to stronger finite-size effects than Z_{2h}, so a weak pairing might still survive for $|t|/t_2>1$.

Since phase separation might compete with superconductivity, one needs now to consider the four-hole binding energy $\Delta_4=E_{4h}+E_{0h}-2E_{2h}$, from which an estimate of the compressibility $\kappa=\partial^2 E/\partial n_h^2$ at small hole density $n_h=N_h/N$ can be given using $\kappa^{-1}\simeq N\Delta_4$. Phase separation signaled by a negative curvature of $E(n_h)$ implies, in this case, the formation of four-hole droplets (quartets), i.e., $\Delta_4<0$. Our numerical calculation of Δ_4 on 32 sites shows that quartets are stable when t is small enough, the plaquette resonance and bond exchange providing an effective "glue" to bind holes together. Such behavior is similar to the case of the doped quantum AF.[20] However, here a very small hopping t can easily suppress phase separation, while affecting pairing only slightly. Indeed, for a typical value of $J/t_2=0.5$, $\Delta_4\simeq -0.0635t_2$ (meaning $\kappa<0$) for static holes ($t=0$) while $\Delta_4\simeq -0.0042t_2$ ($\Delta_4\simeq -0.0011t_2$) for $t=0.1t_2$ ($t=-0.1t_2$) and $\Delta_4\simeq 2.471t_2$ ($\Delta_4\simeq 2.044t_2$) for $t=0.5t_2$ ($t=-0.5t_2$). We therefore expect a paired state when $t/t_2>0.1$.

Lastly, we would like to draw possible scenarios at finite doping. (i) If plaquette ordering survives at sufficiently small doping (plausible since the RSPC is "protected" by a finite

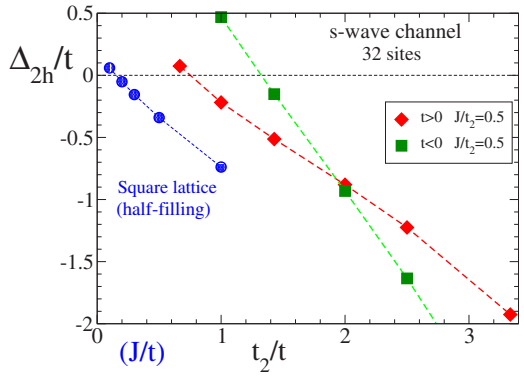

FIG. 5. (Color online) Hole pair binding energy (in units of t) vs $t_2/|t|$ for both signs of t. For comparison, the case of the doped quantum AF on the square lattice is shown (data for $N=26$) (Ref. 19).

gap), one expects a superconducting phase which inherits broken translational symmetry from its parent Mott insulator (the RSPC). This can be viewed as a new type of supersolid with no charge modulation.[21] (ii) Alternatively, hole pairs could be arranged along domain walls between out-of-phase RSPC regions. This scenario is, however, unlikely, providing no obvious gain of kinetic energy with respect to the supersolid.

To summarize, on the checkerboard lattice, at quarter filling and in the limit of large NN repulsion (enforcing the ice rule constraint on every tetrahedron), the Hubbard model exhibits a robust insulating resonating singlet-pair crystal with a uniform average charge. We provide arguments for Cooper pair formation and argue in favor of a supersolid phase in an extended region of parameters, phase separation being confined only to very small hole kinetic energy. However, hole Cooper pairs seem to be more fragile for large hopping than in the doped antiferromagnet on the square lattice.

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[11] For two holes (two electrons) doped, the GS $\mathbf{k}=\mathbf{0}$, A_1 (B_1), and time-reversal (TR) -1 irreducible representation contains 9 244 689 (130 840 618) states.

[12] A reduced Brillouin zone (BZ) scheme is used (two-site unit cell). The states are classified according to the A_1, A_2, B_1, B_2, and E irreducible representations of the point group D_4 (origin at the center of an empty square).

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