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Exact Hole-induced Resonating-Valence-Bond Ground State in Certain $U = \infty$ Hubbard Models

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We prove that the motion of a single hole induces the nearest-neighbor resonating-valence-bond (RVB) ground state in the $U = \infty$ Hubbard model on a triangular cactus – a tree-like variant of a kagome lattice. The result can be easily generalized to $t - J$ models with antiferromagnetic interactions $J \geq 0$ on the same graphs. This is a weak converse of Nagaoka’s theorem of ferromagnetism on a bipartite lattice.

A resonating-valence-bond (RVB) state is an exotic spin liquid state originally envisioned by Anderson [1]. It was revisited after the discovery of high T_c superconductivity [2, 3], which gave rise to the notion that by doping the RVB, holons, the fractionalized excitations carrying charge e and spin 0, can condense to become a superconductor [4–6]. In this picture, the background antiferromagnetic interaction, J , plays an essential role as a mediator of valence-bond formation and thus of “preformed Cooper pairs.”

Even in the absence of explicit exchange interactions, however, magnetism can still arise upon doping of the Hubbard model at half-filling in the $U = \infty$ limit (where $J = 0$). The idea is that the motion of a doped hole (or electron) shuffles the background spin ordering, leading to the magnetism [7]. In particular, the celebrated “Nagaoka’s theorem” states that for a bipartite system (e.g. a square lattice), introducing a single hole leads to a fully polarized ferromagnetic ground state due to the constructive interference of the hole motion in a ferromagnetic background [8]. This result was generalized to a wider class of graphs by Tasaki [9] – the only requirement is that the product of hopping matrix elements around any loop in the graph is positive. (See also [10, 11] for a related theme on kinetically induced magnetism.) On a non-bipartite lattice, however, the product of hopping matrix elements around loops with an odd number of bonds is negative, frustrating the kinetic energy of a hole in a ferromagnetic background. Indeed, recent numerical studies have concluded that the ground state of the $U = \infty$ Hubbard model on a triangular lattice in the presence of a single hole has total spin zero ($S_{\text{tot}} = 0$) and has 120° order as in the case of triangular lattice antiferromagnet [12–15].

In this paper, starting from a simple problem on a single triangle, we study the $U = \infty$ Hubbard model on a certain class of graphs known as a triangular cactus (also known as a Husimi cactus), on which the kinetic motion of a hole is unfrustrated (frustrated) in an RVB (ferromagnetic) background. The ground state of this model is rigorously proven to be a nearest-neighbor RVB state with a delocalized holon. Such a graph has a property that the product of hopping matrix elements around any

cycle (a loop of length $l \geq 3$ in which only the first and the last vertices are equal) is *negative*. We also remark that the system is integrable thanks to the existence of extensive number of conserved quantities – this is an example of Hilbert space fragmentation [16–18].

A hole in a triangle. We start by solving the two-electron problem for the Hubbard model on a triangle with $U = \infty$ and $t > 0$:

$$H = -t \sum_{i=1}^3 \sum_{\sigma=\uparrow,\downarrow} \left[c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.} \right] + [U = \infty], \quad (1)$$

where the site $i = 4$ is identified with $i = 1$ ($c_{4,\sigma} \equiv c_{1,\sigma}$). In the total $S = 1$ (triplet) sector, energy eigenvalues are $E_n = 2t \cos(\frac{2\pi n}{3})$, where $n = 0, 1, 2$, with three-fold degeneracies due to the spin-rotational symmetry (corresponding to the total $S^z = \pm 1, 0$). In the $S = 0$ (singlet) sector, energy eigenvalues are $E_n = -2t \cos(\frac{2\pi n}{3})$, where $n = 0, 1, 2$. The ground state is the singlet state:

$$|\text{GS}\rangle = \frac{1}{\sqrt{3}} \left(|\text{triangle with hole at site 1 and magenta bond 1-2}\rangle + |\text{triangle with hole at site 2 and magenta bond 2-3}\rangle + |\text{triangle with hole at site 3 and magenta bond 3-1}\rangle \right), \quad (2)$$

where a circle on a vertex denotes the location of a hole and the magenta bond denotes the singlet state on two sites. The singlet state is oriented in a counter-clockwise direction on a triangle. In the $S = 0$ ground state, the hole’s kinetic energy has its minimum possible value $-2t$, whereas it is frustrated in a spin-polarized background, with the lowest energy being $-t$.

Indeed, in the singlet subspace ($S^2 = 0$), unique basis states can be identified with the location of the holon, i.e. the state $|\text{triangle with hole at site 1 and magenta bond 1-2}\rangle$ can be identified as the state with a holon (with its creation operator $h_i^\dagger$) at the circled site. In the triplet sector ($S = 1$), with a fixed total $S^z = \pm 1, 0$, the basis states can similarly be identified by the position of the hole. It is then easy to see that the Hamiltonian of a hole in the singlet sector is given by $H_{\text{eff}}^{(s)} = -t \sum_{i=1}^3 \left(h_i^\dagger h_{i+1} + \text{H.c.} \right)$, whereas in the triplet sector with a fixed total S^z , $H_{\text{eff}}^{(t)} = +t \sum_{i=1}^3 \left(h_i^\dagger h_{i+1} + \text{H.c.} \right) = -t \sum_{i=1}^3 \left(e^{-i\pi} h_i^\dagger h_{i+1} + \text{H.c.} \right)$. Effectively, the hole sees a π -flux through the triangle when the background spins form a triplet pair [19].

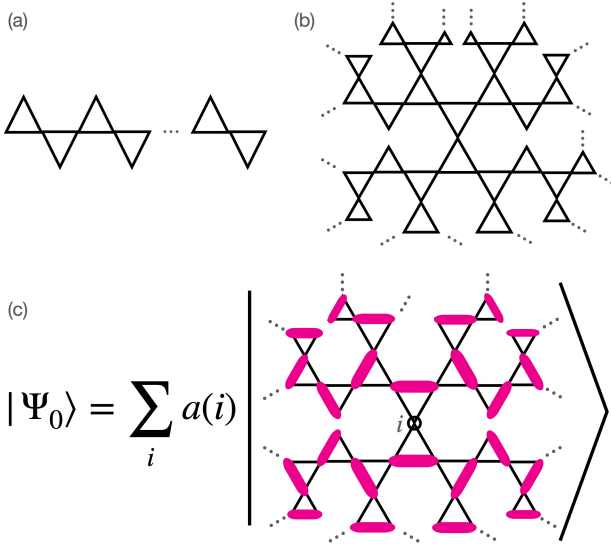


FIG. 1. (a) Sawtooth geometry. (b) An example of a triangular cactus (or a Husimi cactus). It is also possible that three or more triangles share the same vertex. (c) The RVB ground state induced by the hole motion in the $U = \infty$ Hubbard model on the triangular cactus. Here, i denotes the location of the holon (circled) and magenta ellipses indicate singlet valence bonds of two $S = \frac{1}{2}$ spins. The amplitude, $a(i)$, of each valence-bond configuration is all positive, $a(i) > 0$, with the counter-clockwise orientation of valence-bonds as introduced below Eq. 2 & 6.

Triangular cactus. We now consider the *single hole* problem in the $U = \infty$ Hubbard model on a triangular cactus. A triangular cactus is a planar graph where the only cycles – loops of length $l \geq 3$ in which only the first and the last vertices are equal – are triangles and any edge belongs to a cycle. Such a graph has previously been widely studied in the context of spin model (e.g. Heisenberg model) [20–22]. Fig. 1 (a-b) are examples of a triangular cactus. We consider the following $U = \infty$ Hubbard models on such graphs with negative but otherwise arbitrary hopping matrix elements $-t_{ij} < 0$:

$$H = - \sum_{\langle i,j \rangle, \sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + V(\{n_i\}) + [U = \infty]. \quad (3)$$

Here, $\langle i, j \rangle$ denotes the directed bond from the site i to j of the graph, and $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ is the number operator on site i . $t_{ij} \neq 0$ only for those bonds $\langle i, j \rangle$ connected by the triangular cactus. Note that the number of sites i of the graph is always odd ($2N_f + 1$) and the number of *directed* bonds $\langle i, j \rangle$ is $6N_f$, where N_f is the number of plaquettes (or faces) f . $V(\{n_i\})$ denotes arbitrary on-site disorder and interaction terms:

$$V(\{n_i\}) = \sum_i \epsilon_i n_i + \sum_{i,j} V_{ij} n_i n_j + \dots \quad (4)$$

At half-filling (one electron per site), there is a 2^{2N_f+1} spin degeneracy. The main result of the paper (the The-

orem below) is that the motion of a single hole lifts such degeneracy and induces the RVB ground state.

Before going into technical details, we first define the convenient many-body basis of the problem. For this, we make a direct contact with quantum dimer models [4, 23–25], and consider the states of hard-core (nearest-neighbor) dimers on a triangular cactus graph, with a single monomer (that is, all sites but one are touched by a dimer). Once the location of the monomer is specified, it is easy to see that there is a *unique* dimer covering, which has exactly one dimer fully contained in every triangle (see Fig. 1 (c) for the illustration of such a configuration). Now consider the Hamiltonian describing the hopping of a monomer:

$$H_{\text{hop}} = -t \sum_{\triangle} \left(|\triangle\rangle\langle\triangle| + |\triangle\rangle\langle\triangle| + |\triangle\rangle\langle\triangle| + |\triangle\rangle\langle\triangle| + \text{H.c.} \right), \quad (5)$$

where a circle on a vertex denotes the location of monomer. The dimer is colored black to differentiate it from a singlet bond. In any step in which the monomer hops to a nearest-neighbor site, one dimer is moved, but in such a way that it remains interior to the same triangle. *Thus, we can label the dimers uniquely by a plaquette index f , and this index is preserved under the specified dynamics.*

Now let us consider the corresponding electron problem. Given the location of the hole, i , and the corresponding unique dimer covering, let $\tilde{S}_f$ and $\tilde{S}_f^z$ be the total spin and spin component in the z -direction, respectively, of the two electrons touched by the dimer contained in the plaquette f . The two spins form either a singlet or triplet state: $\tilde{S}_f = 0, 1$. $\tilde{S}_f$ and $\tilde{S}_f^z$ constructed in this way form an extensive set of *local* conserved quantities: $[\tilde{S}_f, H] = [\tilde{S}_f^z, H] = 0$ for all f . *Note that $\tilde{S}_f$ and $\tilde{S}_f^z$ are different from S_f and S_f^z , the total spin and the spin in z -direction of the three sites in f .* Finally, we form the following orthonormal basis states:

$$|i, \{\tilde{S}_f\}, \{\tilde{S}_f^z\}\rangle, \quad (6)$$

where $i = 1, 2, \dots, 2N_f + 1$ and $f = 1, 2, \dots, N_f$. *Again, we choose to orient valence-bonds in counter-clockwise direction around each triangle, f , whenever $\tilde{S}_f = 0$.* (This introduces a sign convention for resonating-valence-bond-type wave-functions [26].) Of these basis states, the state corresponding to the unique valence-bond covering with the holon at site i will be denoted by

$$|i, \text{VBC}\rangle \equiv |i, \{\tilde{S}_f \equiv 0\}, \{\tilde{S}_f^z \equiv 0\}\rangle. \quad (7)$$

Then, the following theorem is the main result of this paper.

Theorem: The ground state of the Hamiltonian Eq. 3 in the presence of a single hole ($2N_f$ electrons on $2N_f + 1$

sites) is unique and is the positive ($a(i) > 0$) superposition of all the possible valence-bond coverings $|i, \text{VBC}\rangle$. This is the nearest-neighbor “resonating-valence-bond (RVB) state” with a delocalized holon [27]:

$$|\Psi_0\rangle = \sum_i a(i) |i, \text{VBC}\rangle. \quad (8)$$

(see Fig. 1 (c) for the illustration of this RVB state.)

The Theorem can be easily proven with the following well-known lemma (see e.g., Ref. [28]).

Lemma (diamagnetic inequality): Consider a single particle hopping problem under a magnetic field on a general 2-edge-connected planar graph in the presence of an arbitrary on-site potential term:

$$T[\{\phi_f\}] + V_0 \equiv - \sum_{\langle i,j \rangle} t_{ij} e^{-i\theta_{ij}} |i\rangle \langle j| + \sum_i \epsilon_i |i\rangle \langle i|, \quad (9)$$

where we assume $t_{ij} > 0$ and θ_{ij} is an induced Berry phase on an edge $\langle i, j \rangle$ due to a flux ϕ_f through a plaquette f to which $\langle i, j \rangle$ belongs. We will simply denote by T_0 the hopping matrix in the absence of a magnetic field: $T_0 \equiv T[\{\phi_f \equiv 0\}]$. Here, a 2-edge-connected graph is a connected graph in which every edge belongs to at least one plaquette. Formally, it is defined to be a connected graph that cannot be disconnected by deleting any single edge. Then, the flux configuration that minimizes the ground state energy of $T[\{\phi_f\}]$ is unique and is the one without any flux: $\phi_f = 0$ for all f , i.e. when $T[\{\phi_f\}] = T_0$. The physical meaning is that “a magnetic field raises the energy.”

Proof of the lemma: Let $|\psi'\rangle$ be the normalized ground state of $T[\{\phi_f\}] + V_0$ for a given non-trivial flux configuration $\{\phi_f\}$ with the energy E'_0 , and $|\psi\rangle$ be the normalized ground state of $T_0 + V_0$ with the energy E_0 . It is easy to see that $E_0 \leq E'_0$ by using the triangle inequality:

$$\begin{aligned} E'_0 &= - \sum_{\langle i,j \rangle} t_{ij} e^{-i\theta_{ij}} \psi_i'^* \psi_j' + \sum_i \epsilon_i |\psi_i'|^2 \\ &\geq - \sum_{\langle i,j \rangle} t_{ij} |\psi_i'| \cdot |\psi_j'| + \sum_i \epsilon_i |\psi_i'|^2 \\ &= \langle |\psi'| | (T_0 + V_0) | |\psi'| \rangle \geq E_0. \end{aligned} \quad (10)$$

Here, $|\cdot|$ denotes the matrix with every entry replaced by its absolute value: e.g., $(|A|)_{ij} \equiv |A_{ij}|$.

In order to prove the uniqueness, it is enough to show that the first inequality above is a strict inequality. Let us assume otherwise, in which case each term in $-\langle \psi' | T[\{\phi_f\}] | \psi' \rangle$ is real and positive:

$$e^{-i\theta_{ij}} \psi_i'^* \psi_j' > 0 \quad (11)$$

for all $\langle i, j \rangle$. Now, let $\phi_f \neq 0$ for some plaquette f , with its vertices $i_1, i_2, \dots, i_n$ ($i_{n+1} \equiv i_1$). From Eq. 11, we obtain

$$\prod_{k=1}^n e^{-i\theta_{i_k i_{k+1}}} \psi_{i_k}'^* \psi_{i_{k+1}}' = e^{-i\phi_f} \prod_{k=1}^n |\psi_{i_k}'|^2 > 0, \quad (12)$$

which is in contradiction to the assumption that $\phi_f \neq 0$. This completes the proof. $\square$

Proof of the Theorem: Since $[\tilde{S}_f, H] = [\tilde{S}_f^z, H] = 0$, let us consider the Hamiltonian Eq. 3 in a given $\{\tilde{S}_f\}$ and $\{\tilde{S}_f^z\}$ sector, $H|_{\{\tilde{S}_f\}, \{\tilde{S}_f^z\}}$. As shown in the single triangle problem above, the hole sees effective π -fluxes (no-fluxes) on triangles, f , at which $\tilde{S}_f$ is a triplet (singlet). Hence, $H|_{\{\tilde{S}_f\}, \{\tilde{S}_f^z\}}$ is the Hamiltonian of a single hole hopping problem in the presence of π -fluxes through the triangle plaquettes, f , with $\tilde{S}_f = 1$. According to the lemma (diamagnetic inequality), the energy minimizing flux configuration is unique and is the one without any flux, and hence, $\tilde{S}_f = 0$ and $\tilde{S}_f^z = 0$ for all f . Also,

$$H|_{\{\tilde{S}_f=0\}, \{\tilde{S}_f^z=0\}} = - \sum_{\langle i,j \rangle} t_{ij} |i\rangle \langle j| + \sum_i \tilde{V}_i |i\rangle \langle i|, \quad (13)$$

where $\tilde{V}_i \equiv V(\{n_i = 0, n_{j \neq i} = 1\})$ is the effective on-site potential felt by the hole at site i . Since the off-diagonal elements of $H|_{\{\tilde{S}_f=0\}, \{\tilde{S}_f^z=0\}}$ are all negative, the Perron-Frobenius theorem ensures that the ground state, $|\Psi_0\rangle$, of $H|_{\{\tilde{S}_f=0\}, \{\tilde{S}_f^z=0\}}$ (and hence of H) is the superposition of all the basis states (Eq. 7) with positive coefficients, Eq. 8. $\square$

t - J model. The nearest-neighbor RVB state of the form Eq. 8 with $a(i) > 0$ is still a ground state in the presence of nearest-neighbor antiferromagnetic Heisenberg interactions, $J > 0$ of the following form:

$$\begin{aligned} H_J &= \sum_f J_f \sum_{l=1}^3 \tilde{S}_l^{(f)} \cdot \tilde{S}_{l+1}^{(f)} \\ &= \sum_f \frac{J_f}{2} \left[S_f(S_f + 1) - \frac{3}{4} n_f \right]. \end{aligned} \quad (14)$$

Here, $\tilde{S}_l^{(f)} = \sum_{s,s'=\uparrow,\downarrow} c_{l,s}^\dagger \frac{\vec{\sigma}_{ss'}}{2} c_{l,s'}$ ($l = 1, 2, 3$) is the spin operator on site l of a triangle f (with $S_4^{(f)} \equiv S_1^{(f)}$), $\tilde{S}_f = \sum_{l=1}^3 \tilde{S}_l^{(f)}$, and n_f is the total number operator on a triangle f . Antiferromagnetic interactions J are uniform for bonds of the same triangle f , while they can differ on different triangles.

Proof of the Theorem in the presence of $J \geq 0$: Observe that each $|i, \text{VBC}\rangle$ describing a valence-bond covering with the holon at site i is an eigenstate of H_J with the lowest possible energy eigenvalue (for a fixed i):

$$H_J |i, \text{VBC}\rangle = \left(-\frac{3}{4} \sum_f J_f \right) |i, \text{VBC}\rangle. \quad (15)$$

This means that the ground state of the total Hamiltonian including H_J is still in the $\{\tilde{S}_f = 0\}$ sector. Moreover, since $H_J|_{\{\tilde{S}_f=0\}, \{\tilde{S}_f^z=0\}}$ is diagonal in the basis $|i, \text{VBC}\rangle$, it follows from the Perron-Frobenius theorem

that the ground state is still of the form Eq. 8, with $a(i)$ modified but remaining positive. $\square$

Integrability. When $J = 0$ (i.e., $H_J = 0$), the entire excited state spectra of Eq. 3 can be obtained by exploiting the extensive set of quantum numbers $\{\tilde{S}_f\}$ and $\{\tilde{S}_f^z\}$ ($f = 1, 2, \dots, N_f$). The spin excitations are $\tilde{S}_f = 1$ triplets localized on certain triangles f . Let us denote by Δ_s (Δ_t) the set of directed bonds of triangles at which $\tilde{S}_f$ forms a singlet (triplet). The charge spectrum can be obtained by diagonalizing the single hole problem in the presence of π -fluxes on Δ_t [29]:

$$H|_{\{\tilde{S}_f\}, \{\tilde{S}_f^z\}} = - \sum_{\langle i, j \rangle \in \Delta_s} t_{ij} |i\rangle \langle j| - \sum_{\langle i, j \rangle \in \Delta_t} t_{ij} e^{-i\pi} |i\rangle \langle j| + \sum_i \tilde{V}_i |i\rangle \langle i|. \quad (16)$$

In the presence of H_J , $\tilde{S}_f$ and $\tilde{S}_f^z$ are no longer good quantum numbers, and the system is no longer integrable.

Relevance of the sign of hopping matrix elements. In the presence of the uniform π -flux on each triangle, which amounts to changing the sign of hopping terms $t_{ij} \rightarrow -t_{ij}$, the ground state manifold consists of the states with N_f uncorrelated spin triplets, each of which is localized on the triangle f :

$$|\{\tilde{S}_f^z\}\rangle \equiv \sum_i b(i) |i, \{\tilde{S}_f = 1\}, \{\tilde{S}_f^z\}\rangle, \quad (17)$$

where $b(i) > 0$ and $\{\tilde{S}_f^z\} = \pm 1, 0$. The ground states are 3^{N_f} -fold degenerate; among them is the familiar fully-polarized Nagaoka ferromagnet. If the π -fluxes are present only in some $N_\phi (< N_f)$ number of triangles, the ground state manifold consists of the states with localized triplets $\tilde{S}_f = 1$ on those N_ϕ triangles and is 3^{N_ϕ} -fold degenerate.

Spin- $\frac{1}{2}$ bosons. All of the above conclusions remain true for spin- $\frac{1}{2}$ hard core bosons if the sign of the hopping term is reversed. This is a weak converse to the results of Ref. [30, 31] which show that the ground state of spin- $\frac{1}{2}$ bosons is a fully-polarized ferromagnet when the hopping matrix elements are all negative.

Discussion. The exact solvability of the present model relies on its “tree-like” structure, i.e. due to the absence of loops other than triangles. Exact generalization of this result to a 2D or higher dimensional lattice is likely to be obstructed by the existence of longer-ranged valence-bonds generated by the hopping of a holon around an additional loop adjacent to a certain triangle. Moreover, the existence of additional even-length loops produces a tendency towards a ferromagnetism, as exemplified by the Nagaoka’s theorem on a bipartite lattice, and frustrates a tendency to a singlet formation, making analytic solution highly unlikely. However, if the number of non-triangular loops is suppressed in comparison to the number of (corner-sharing) triangles, it is likely that a version

a short-ranged RVB state is stabilized: a kagome lattice or a suitably decorated version of it may be such an example. Such an idea is in line with the attempts to reproduce quantum dimer models as a limiting case by suitably decorating each edge of 2D lattices with Majumdar-Ghosh chain [32, 33].

We hope that the present exact result will prove to be a fruitful starting point for a numerical search for a doping-induced RVB state (as opposed to doping an RVB state induced by frustrated antiferromagnetic interactions). In particular, a numerical study of the $U = \infty$ Hubbard model on a kagome lattice is currently lacking, although such studies have been carried out for the square and triangular lattices [15, 34]. Whether doping dilute holes in the $U = \infty$ Hubbard model on the kagome lattice leads to superconductivity [35–38], a holon Fermi liquid, a holon Wigner crystal [39], or some other state is an interesting open question.

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