

Magnetization of Electronic Ground States in Frustrated Superstable Graphs

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Geometric frustration lies at the heart of many unconventional quantum phases in strongly interacting electron systems. Here, we analytically determine the ground state magnetization of the half-filled Hubbard model on frustrated geometries where superstable states—eigenstates which are robust against frustration—are manifest. Our results apply to a broad class of lattices, including those where altermagnetic and superconducting states are known to emerge. Furthermore, they provide evidence for phase transitions involving a geometric rearrangement of magnetic correlations in the thermodynamic limit.

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Introduction—Magnetic frustration gives rise to many exotic phenomena in many-body physics, and is of fundamental importance in spintronics [1–11]. For instance, recent work has predicted flat band physics in a plethora of frustrated lattices [12] and materials with a Kagome lattice structure have shown evidence of intertwining between superconducting, density wave and spin liquid phases [13]. In quasi-1D systems described by zigzag chains [14–17], frustration may be responsible for the spin-Peierls transitions witnessed in, e.g., TTF-CuS₄C₄(CF₃)₄ and CuGeO₃ [18–20], while the Shastry-Sutherland lattice [21–24] is predicted to feature altermagnetism and could be realized, e.g., in α - or κ -(BEDT-TTF)₂X charge transfer salts [25]. Charge transfer salts with other frustrated geometries also exhibit superconductivity, Mott physics, and putative spin liquid phases [26,27]. These results highlight the richness of frustrated quantum materials and motivate the development of numerical and analytical approaches to identifying the ground state properties of the corresponding many-body Hamiltonian.

In this regard, the Hubbard model and its exact [28–34] and numerical [35–38] treatments have played an outstanding role. Despite its apparent simplicity, the Hubbard model and extensions thereof qualitatively capture a wide range of many-body phenomena observed in highly distinct

classes of quantum materials [39,40]. These include Mott-insulating phases, high-temperature superconductivity [41–44], light-induced superconductivity [45–50], nontrivial topological properties [51,52], and magnetic order [53–57]. Notably, exact results have revealed how magnetism in the ground state is intimately tied to the underlying graph that encodes the lattice geometry, hopping amplitudes, and electron filling [58–66]. In the half-filled case, these results apply only to bipartite graphs [58,59]. Specifically, Lieb’s theorem [58] guarantees uniqueness and determines the magnetization of the ground state in Hubbard models on such graphs, while the Shen-Qiu-Tian theorem [59] shows that this state exhibits ferrimagnetic correlations. Yet, as highlighted, many important systems lack a bipartite lattice structure, giving rise to geometrical frustration [67].

In this Letter, we extend Lieb’s and Shen-Qiu-Tian’s theorems within the strongly correlated regime of the half-filled Hubbard model to a broad class of nonbipartite graphs. In this limit of strong Coulomb repulsion, ground state properties may be deduced analytically from an associated spin Hamiltonian, which exhibits superstable ground states. These are eigenstates of the associated spin Hamiltonian, originally introduced by Shastry and Sutherland [68], for which frustrating couplings exactly vanish. We refer to graphs that give rise to such superstable ground states in the associated spin Hamiltonian as superstable graphs. Figure 1 shows notable examples of superstable graphs, including the zigzag and Shastry-Sutherland lattices, where the magnetic properties of the ground state of the Hubbard model are obtained via an effective Heisenberg Hamiltonian. In contrast, other superstable graphs—including the diamond chain [69–71] and the

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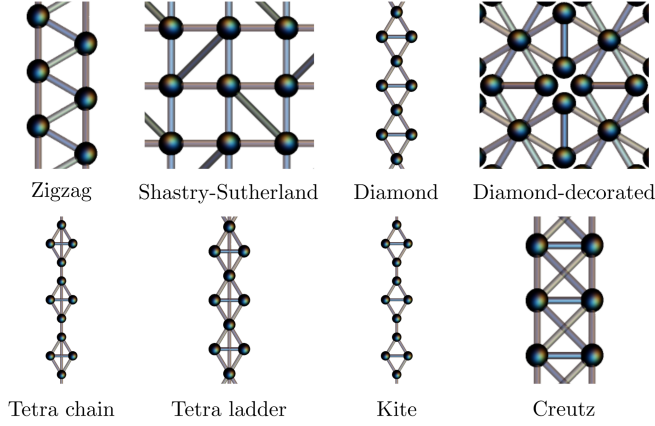


FIG. 1. Quasi-one-dimensional and two-dimensional examples of frustrated superstable graphs. Zigzag chains [20], as realized e.g. in $\text{TTF-CuS}_4\text{C}_4(\text{CF}_3)_4$ and CuGeO_3 . The Shastry-Sutherland lattice, expected to be realized in α - or κ -(BEDT-TTF) $_2\text{X}$ [25]. Examples of diamond-shaped compounds are $\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$, $\text{K}_3\text{Cu}_3\text{AlO}_2(\text{SO}_4)_4$ and $\text{Cu}_3(\text{CH}_3\text{COO})_4(\text{OH})_2 \cdot 5\text{H}_2\text{O}$ [77–79]. Reference [12] reports that, in total, more than two thousand known materials have diamond, tetra chain, tetra ladder, kite, or Creutz geometries.

diamond-decorated square lattice [72–76]—require incorporating additional charge fluctuations, as the Heisenberg model alone fails to reproduce the magnetic properties.

As an application of our results, we study the Hubbard model on a diamond chain. This graph can be tuned from a bipartite to a frustrated regime where a superstable ground state emerges in the associated spin model. In the thermodynamic limit, this crossover develops into a first-order phase transition, a behavior that may reflect a more general characteristic of ground state phase diagrams of superstable graphs. We envision that our *analytical* results may guide the search for systems with topological spin textures or the study of superconducting condensation in driven quantum materials.

Results—We study magnetism in Hubbard models on weighted graphs [see Fig. 2(a)]. A weighted graph $G = (V, E, t(E))$ is a set of vertices V , a set of edges E which correspond to pairs of vertices (i, j) with $i \neq j$ and $i, j \in V$, and weights $t(e)$ which maps edges $e \in E$ into nonzero scalars. For the Hubbard model, the weights represent the hopping amplitude between pairs of sites. The Hubbard model on a weighted graph thus reads,

$$H(G) = U \sum_{i \in V} n_{i,\uparrow} n_{i,\downarrow} - \sum_{e=(i,j) \in E} \sum_{\sigma} t(e) \left(c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.} \right), \quad (1)$$

where $n_{i,\uparrow}$, $c_{i,\sigma}$, $c_{i,\sigma}^\dagger$ are the fermionic number, annihilation, and creation operators at vertex $i \in V$ with spin $\sigma \in \{\uparrow, \downarrow\}$. The interaction $U > 0$ accounts for the local Coulomb

repulsion. The Hamiltonian has a $\text{SU}(2)$ global spin rotation symmetry as it commutes with all the total spin operators $S^\alpha = \sum_{i \in V} S_i^\alpha$ where $S_i^\alpha = \sum_{\sigma, \sigma'} c_{i,\sigma}^\dagger (\sigma^\alpha)_{\sigma\sigma'} c_{i,\sigma'}$ with σ^α the Pauli matrices and $\alpha \in \{x, y, z\}$ [80]. This symmetry allows the characterization of every eigenstate of the Hubbard Hamiltonian with a total spin S , which can take positive integer or half-integer values.

At half filling, in the strongly correlated regime [i.e., $U \gg \max(|t(e)|)$, see End Matter (EM)], the ground state magnetic properties of Eq. (1) can be obtained from effective spin models derived via a Schrieffer-Wolff (SW) transformation expansion up to order n in U^{-1} [81,82]. The $n = 1$ order gives $H_H(G_H)$; the spin-1/2 Heisenberg Hamiltonian on the weighted graph $G_H := (V, E, 4t(E)^2/U)$ (i.e., the parent graph with transformed weights) and $H_H(G) := \sum_{e=(i,j) \in E} t(e) (\vec{S}_i \cdot \vec{S}_j - 1/4)$. This effective model is known to capture the magnetic properties of Hubbard models on connected bipartite graphs [34,83]. A graph is bipartite if we can define disjoint sets A and B such that $A \sqcup B = V$ and for every edge $e = (i, j) \in E$, we have $i \in A$ and $j \in B$. According to Lieb’s, Lieb-Mattis’s, and Shen-Qiu-Tian’s theorems, this partition of vertices determines the total spin of both models as $S = (||A| - |B||)/2$ [58,84] and the sign of their ground state magnetic correlations [59,85], $\langle S_i^+ S_j^- \rangle$, where $S_i^\pm = S_i^x \pm iS_i^y$. In other words, these theorems map the problem of finding the ground state magnetic properties to a simple graph theory problem—finding the bipartition.

In contrast to the bipartite case, higher orders of the SW transformation expansion may be necessary to capture the magnetic properties of the Hubbard model on frustrated graphs. At these higher orders, the resulting spin models do not “live” on the same graph as the parent Hubbard model: they generically feature new pairwise interactions that add edges to the parent graphs, altering their geometry, and they also include beyond-pairwise interactions that cannot be represented as edges [86]. However, on superstable graphs, those frustrating and beyond-pairwise interactions vanish (see EM), and the ground state magnetic properties can be found from effective spin models on bipartite graphs. Hence—in the same spirit as the previous theorems—determining magnetic properties on superstable graphs reduces to finding effective bipartite graphs.

To see how this occurs, consider the $n = 1$ order of the SW transformation expansion of the superstable graph in Fig. 2(a): a diamond composed of a vertical dimer uniformly coupled ($t_{1,3} = t_{2,3}$ and $t_{1,4} = t_{2,4}$) to residual vertices (3 and 4) that introduce frustration [see Fig. 2(b)]. Due to the uniform coupling, the frustrating spin interactions are proportional to the total spin of the dimer, $S_1^\alpha + S_2^\alpha$, and thus vanish when it forms a singlet, $|0\rangle_C := (|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2) / \sqrt{2}$. Consequently, the states $|0\rangle_C \otimes |\sigma\rangle_3 \otimes |\sigma'\rangle_4$ are said to be superstable to the frustrating terms [68]. When $t_{1,2}$ is sufficiently large, these

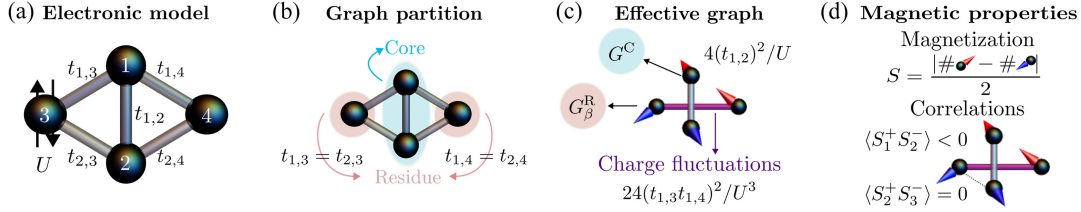


FIG. 2. (a) Sketch of a Hubbard model on a single diamond with hopping weights $t_{i,j} := t(e)$ with $e = (i, j)$ where i and j are vertices of the graph and on-site repulsion U . (b) The graph is partitioned into a core (formed by a dimer in this example) and a residue, identified through relations between the hopping weights. (c) The graph partition defines two bipartite graphs— G^C and G^R_β —in an effective spin model, obtained in the strongly correlated regime. When the ground state of the effective model is superstable, couplings causing geometric frustration vanish. Consequently, the bipartition of G^C and G^R_β determines the ground state properties. The horizontal coupling connecting the vertices in G^R_β is not present in the original graph; it is mediated by charge fluctuations arising from higher-order corrections, with weights parametrized by a hopping-anisotropy β . (d) The ground state magnetization, S , and the sign of the magnetic correlations, $\langle S_i^+ S_j^- \rangle$, of the Hubbard model are given by the partition of the effective graph.

become ground states with $S = 0$ and 1, corresponding to a singlet or a triplet on the residual vertices, respectively. However, charge fluctuations from the $n = 3$ order of the SW transformation expansion break this degeneracy in the Hubbard model as they mediate an antiferromagnetic coupling $\sim t_{1,3}^2 t_{1,4}^2 / U^3$ between the residual vertices, thereby forming an effective dimer on sites 3 and 4, and energetically favor its singlet state [see Fig. 2(c)]. Hence, the $n = 3$ corrections stabilize a unique superstable ground state with $S = 0$. Due to the superstable property of the ground state, the magnetization of this state can be thought of as the sum of the ground state magnetization of two independent dimers. We thus see that the ground state magnetic properties of the frustrated graph in Fig. 2(a) are found from the analysis of a Heisenberg Hamiltonian on a different bipartite graph, as shown in Fig. 2(d).

This simple approach generalizes to a broader class of superstable graphs. Importantly, in the EM, we introduce an algorithm based on established graph theory concepts, such as modular decomposition [87,88], that systematically identifies graphs that show superstable ground states in the $n = 1$ or $n = 3$ order. Given a superstable graph, the algorithm returns two effective bipartite graphs: a core graph G^C —generalizing the first dimer—whose connected components [89] form connected bipartite and balanced (i.e., $|A| = |B|$) graphs, and a residue graph G^R_β —built from the residual vertices and the effective edges created by charge fluctuations—which contains at most one unbalanced connected component. In the single-diamond example above, G^R_β is the dimer on sites 3 and 4. The weights of the residue graph depend on the hopping-anisotropy $\beta := \{\max_{e \in E \setminus E^C} [|t(e)|] / \min_{e \in E^C} [|t(e)|] \}^2$, with E^C the set of edges of G^C . Physically, the hopping-anisotropy controls how strongly the residue frustrates the core singlets. In the single-diamond example above, $\beta = \{\max(|t_{1,3}|, |t_{1,4}|) / |t_{1,2}|\}^2$, so small β corresponds to a strongly bound vertical dimer, stabilizing its singlet and

effectively decoupling it from the residual vertices. We emphasize that this residue graph contains the new edges added by charge fluctuations [see Fig. 2(c)], which depend on the geometry of the parent graph (see EM). The bipartition of these graphs determines the ground state magnetic properties, as given by our main results:

Theorem 1—If a graph is superstable, then, in the strongly correlated regime, for sufficiently small β , every ground state has total spin $S = (||A| - |B||)/2$. The ground states are exactly $(2S + 1)$ -fold degenerate. Here, $A \sqcup B$ is the bipartition for the only unbalanced component of G^R_β . If all are balanced, $S = 0$.

Here, as above, the strongly correlated regime means that U is large enough so that the gap of a unique ground state (up to the trivial degeneracy) of the order- n SW effective spin Hamiltonian is not closed by higher-order corrections. Thus, the total S predicted by this ground state is the same as that of the Hubbard model. This regime always exists; see the EM for the formal statements. The trivial $2S + 1$ degeneracy comes from the $SU(2)$ invariance of the model, which guarantees that each eigenenergy is at least $(2S + 1)$ -fold degenerate. Therefore, the ground states are unique apart from this mandatory spin degeneracy. Note that the total magnetization is given by the sole unbalanced component of the residue graph. As all other components of the effective graphs are balanced, they cannot contribute to the total magnetization.

Under the same conditions of Theorem 1, ferrimagnetic correlations [34] appear within the individual components of the effective graphs. Formally, this statement is expressed by the following corollary.

Corollary 1 (Approximate ferrimagnetism)—Within the bipartition of each component of G^C and G^R_β , up to $1/U^2$ corrections, the magnetic correlations, $\langle S_i^+ S_j^- \rangle$, are positive (negative) when i belongs to the same (opposite) disjoint partition as j and zero when i and j belong to different components.

The proofs of the theorem and corollary are in the EM.

Applications—Although the emergence of a superstable ground state in the effective spin model might seem uncommon at first glance, important lattice structures host this property. For example, bipartite graphs are naturally superstable (there is no frustration), and Theorem 1 reduces to Lieb’s theorem. In this case, Theorem 1 applies to any $U > 0$ [58], the parameter β can have any positive value, the graph G^C is empty, and $G_\beta^R = G_H$. Under the same conditions, Corollary 1 reduces to the Shen-Qiu-Tian theorem [59], where the corrections are exactly zero. Thus, our results correctly reproduce the ferrimagnetism of bipartite graphs through the $n = 1$ expansion. Meanwhile, the properties of the zigzag chain [14–16] and the Shastry-Sutherland lattice [25] are also described by this expansion order, representing the first set of graphs where our analytical results go beyond Lieb’s and Shen-Qiu-Tian theorems. For these lattices, all vertices are part of a diagonal dimer, which together form G^C . Instead, the graph G_β^R is empty, and Theorem 1 yields $S = 0$. This result, together with Corollary 1, predicts that the dimerization observed in Heisenberg models [15,22] on these geometries also occurs in the Hubbard model.

Furthermore, several candidate flat-band materials, where Hubbard physics is expected to dominate, may also host superstable ground states, provided that the hopping anisotropy is sufficiently small, as their lattice structures are described by superstable graphs. Reference [12] identifies, inter alia, the twelve most prevalent frustrated flat-band lattices among more than 100 000 materials from the Materials Project database [90]. We have identified that five of these nonbipartite structures (i.e., the diamond, tetra chain, tetra ladder, kite, and the Creutz ladder graphs in Fig. 1) are superstable graphs, corresponding to more than 2 000 known materials with the potential to host superstable ground states.

In the following, we explore the Hubbard model on one of these common lattices, the diamond chain, where we need to resort to $n = 3$ to appropriately describe the

magnetic properties. Our results explain density matrix renormalization group (DMRG) simulations of the ground state of the model [91,92]. The vertex labeling is shown in Fig. 3(a). For simplicity, we assume that all the vertical edges have weights t_C and the diagonal edges have nonzero weights t_R . For nonzero t_C , the hopping anisotropy is $\beta = (t_R/t_C)^2$, each pair of vertices coupled with a vertical hopping constitutes a core, and the centered sites are the residual vertices. Figure 3(b) shows the total spin and different ground state regimes of the model obtained from converged DMRG calculations. The crossover between distinct regimes is identified in our simulations by discontinuities in the first derivative of the energy with respect to the ratio t_C/t_R . The insets illustrate typical magnetic correlations within each regime.

Regime I, occurring at $t_C/t_R \gtrsim 1.34$, is the superstable regime, where Theorem 1 and Corollary 1 determine the magnetic properties. The sketch of the effective bipartite graph for this regime is shown in Fig. 3(c). From the sketch, we see that the diagonal edges of the parent graph, which frustrate the vertical dimers, are removed by the superstable ground state. Consequently, this creates disconnected vertical dimers in the effective graph, which together form the graph G^C . The nonzero horizontal weights in the effective spin model are added by the $n = 3$ order of the SW transformation expansion. They create a balanced one-dimensional chain composed of the residual vertices (G_β^R). Since all the connected components of the effective graph are balanced, the total spin is 0 according to Theorem 1. The sign of the numerically obtained correlations agrees with the predictions of Corollary 1 applied to the sketched graph: the one-dimensional chain is disconnected from the dimers (and vice versa), and the correlations are antiferromagnetic within the connected components of the obtained graph. Thus, these results illustrate that the magnetic correlations behave as a composite of ferrimagnetic contributions from the connected

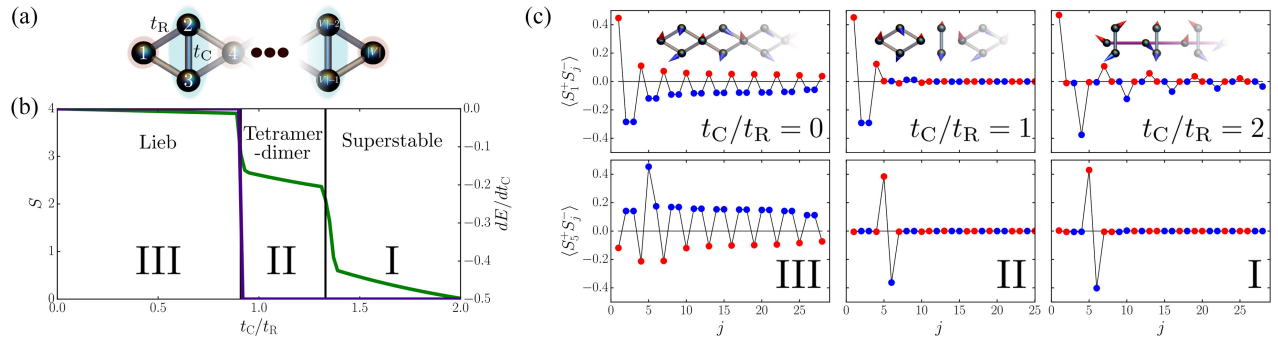


FIG. 3. (a) Diamond chain of $|V|$ vertices and its partitioning into cores (vertical shading) and residue (circles). The weights of the vertical (diagonal) hoppings are given by t_C (t_R). (b) Ground state total spin S (purple line) and first derivative of the energy dE/dt_C (green line) of the Hubbard model on the diamond chain as a function of the strength of the hopping ratio t_C/t_R . The vertical lines mark changes in the ground state characteristics, separating three ground state regimes. (I) The superstable regime is directly described by our results. (II)-(III) The tetramer-dimer and Lieb regimes are related to our results through adiabatic continuation. (c) Representative correlations in the three regimes. The insets show the effective bipartite graph that describes the magnetization and correlations in each regime. The parameters are $|V| = 28$ and $U = 6t_R$.

components. Note that the expansion to $n = 3$ is crucial here: at $n = 1$, the SW transformation gives the Heisenberg model on a diamond chain (with the weights determined by G_H), which is known to show superstable ground states for sufficiently small β [68,70,71]. These states are described by the ground state of the Heisenberg model on a bipartite graph with vertical dimers, but the residual vertices are completely isolated from any other vertex, as in our example of the single diamond. Consequently, $n = 1$ gives highly degenerate (proportional to the system size) ground states, which would result in a paramagnetic response of the system to an external magnetic field, whereas $n = 3$ correctly predicts antiferromagnetism. The latter shows explicitly how the Heisenberg model predicts incorrect physics for frustrated superstable graphs, as it ignores charge fluctuations that lift the ground state degeneracy.

The other two regimes are understood via adiabatic continuation [93] between the ground state of $H(G)$ and the superstable ground state of the Hubbard model on another superstable graph, G' [82]. The graph G' that enables the adiabatic continuation in regime II is obtained by removing every second vertical edge [82]. The resulting superstable ground state eliminates diagonal edges connected to the vertical dimers, leading to a balanced effective graph composed of intercalated tetramers (diamond-shaped bipartite formations of four vertices) and dimers, as shown in the sketch for the corresponding regime in Fig. 3(c). Analogously, for regime III, the superstable graph G' is bipartite and obtained by removing all vertical edges (i.e., setting $t_C = 0$) [82]. Remarkably, we observe that Theorem 1 and Corollary 1, applied to the effective graphs obtained through adiabatic continuation, correctly predict the magnetization and the sign of the numerically obtained correlations, although these results only apply directly to regime I.

The three regimes were shown to converge into ground state phases separated by first-order quantum phase transitions in the thermodynamic limit in Ref. [49]. The emergence of such first-order quantum phase transitions is rooted in Lieb's theorem and Theorem 1. At $t_C = 0$ the graph is connected bipartite, and Lieb's theorem determines $S \propto L/2$ (L is the number of unit cells) as each unit cell is unbalanced due to a single vertex. Instead, the ground state magnetization is $S = 0$ in the superstable regime (assuming an even number of unit cells) as the effective spin model describes a balanced one-dimensional chain with disconnected balanced dimers. Since the ground states belong to two different symmetry sectors, these results imply the existence of at least one ground state energy level crossing at a given system size as t_C/t_R increases. As shown for the diamond chain, there are two energy level crossings from Lieb's regime to the superstable regime. These crossings prevail when increasing the system size and lead to first-order quantum phase transitions.

Beyond the diamond chain, such a level crossing will emerge whenever a hopping-anisotropy ratio analogous to

t_C/t_R interpolates between a bipartite and a superstable regime. Specifically, provided that the total spin predicted by Lieb's theorem in the bipartite regime and Theorem 1 in the superstable regime differ, for sufficiently large U , there is at least one ground state energy level crossing as a function of the hopping-anisotropy ratio. This energy level crossing is expected to give rise to a quantum phase transition [94,95], which need not be first-order, provided that a notion of increasing system size can be defined on the superstable graph, and that the superstable regime remains finite and converges in the thermodynamic limit.

Conclusions—Our results offer new analytical insights into the magnetic properties of frustrated correlated itinerant electron systems and the emergence of quantum phase transitions in the thermodynamic limit. Specifically, we have demonstrated the existence of a ground state regime where the ground state magnetization and ferrimagnetic correlations of a relevant class of frustrated lattices (i.e., with example applications in altermagnetism, flat-band physics, etc.) are determined from a bipartite graph. In this regime, charge fluctuations can become crucial in shaping the magnetic properties as they lift degeneracies. This mechanism has been shown to stabilize topological spin textures in itinerant magnetic systems [96], suggesting that similar topological features may be identified in frustrated geometries with our results or even induced through photoinduced frustration modulation [97].

Our findings are further important for the study of driven quantum materials more broadly [98], since ferrimagnetic ground states were recently identified as promising candidates for optically inducing superconducting condensation in a maximum entropy state upon driving [48]. In this context, superstable states allow a straightforward interpretation of the simulations in [49], as well as the observations of transient superconducting signals in [45,50]. Hence, our results can guide both the development of a symmetry-based theoretical understanding of these phenomena and the search for new opportunities for optical control.

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Data availability—There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

- [1] J. Schulenburg, A. Honecker, J. Schnack, J. Richter, and H.-J. Schmidt, Macroscopic magnetization jumps due to independent magnons in frustrated quantum spin lattices, *Phys. Rev. Lett.* **88**, 167207 (2002).
- [2] J. Richter, Localized-magnon states in strongly frustrated quantum spin lattices, *Low Temp. Phys.* **31**, 695 (2005).
- [3] J. Richter, O. Derzhko, and A. Honecker, The sawtooth chain: From Heisenberg spins to Hubbard electrons, *Int. J. Mod. Phys. B* **22**, 4418 (2008).
- [4] A. Otsuka, D. V. Konarev, R. N. Lyubovskaya, S. S. Khasanov, M. Maesato, Y. Yoshida, and G. Saito, Design of spin-frustrated monomer-type C_{60} - Mott insulator, *Crystals* **8**, 115 (2018).
- [5] H. Diep, *Frustrated Spin Systems* (World Scientific, Singapore, 2004), 10.1142/5697.
- [6] J. Wen, S.-L. Yu, S. Li, W. Yu, and J.-X. Li, Experimental identification of quantum spin liquids, *npj Quantum Mater.* **4**, 12 (2019).
- [7] M. Xu, L. H. Kendrick, A. Kale, Y. Gang, G. Ji, R. T. Scalettar, M. Lebrat, and M. Greiner, Frustration- and doping-induced magnetism in a Fermi–Hubbard simulator, *Nature (London)* **620**, 971 (2023).
- [8] V. Ukleev *et al.*, Frustration-driven magnetic fluctuations as the origin of the low-temperature skyrmion phase in $\text{Co}_7\text{Zn}_7\text{Mn}_6$, *npj Quantum Mater.* **6**, 40 (2021).
- [9] A. O. Leonov and M. Mostovoy, Multiply periodic states and isolated skyrmions in an anisotropic frustrated magnet, *Nat. Commun.* **6**, 8275 (2015).
- [10] J. F. Nossa, M. F. Islam, M. R. Pederson, and C. M. Canali, Electric control of spin states in frustrated triangular molecular magnets, *Phys. Rev. B* **107**, 245402 (2023).
- [11] V. H. González, A. Litvinenko, R. Khymyn, and J. Åkerman, Global biasing using a hardware-based artificial Zeeman term in spinwave Ising machines, *Appl. Phys. Lett.* **124**, 092409 (2024).
- [12] P. M. Neves, J. P. Wakefield, S. Fang, H. Nguyen, L. Ye, and J. G. Checkelsky, Crystal net catalog of model flat band materials, *npj Comput. Mater.* **10**, 39 (2024).
- [13] Y. Wang, H. Wu, G. T. McCandless, J. Y. Chan, and M. N. Ali, Quantum states and intertwining phases in kagome materials, *Nat. Rev. Phys.* **5**, 635 (2023).
- [14] W. J. Caspers, K. M. Emmett, and W. Magnus, The Majumdar-Ghosh chain. Twofold ground state and elementary excitations, *J. Phys. A* **17**, 2687 (1984).
- [15] S. R. White and I. Affleck, Dimerization and incommensurate spiral spin correlations in the zigzag spin chain: Analogies to the Kondo lattice, *Phys. Rev. B* **54**, 9862 (1996).
- [16] T. Onimaru, Y. Ohmagari, S. Mizutani, R. Yamamoto, H. Kaneshima, C. Moriyoshi, D. T. Adroja, D. Khyalyavin, P. Manuel, H. Saito, and C. Hotta, Incommensurate quantum magnet based on 4f-electron in a zigzag spin-1/2 chain of YbCuS_2 , *arXiv:2501.04533*.
- [17] S. Nandi, M. Jawale, S. Bachhar, R. Kumar, M. Schuller, R. Bag, J. Wilkinson, J. Sichelschmidt, A. Sundaresan, S. Haravifard, N. Büttgen, and A. V. Mahajan, Observation of the dimer-singlet phase in the one-dimensional $s = 1/2$ Heisenberg antiferromagnetic $\text{Cu}(\text{Ampy})\text{ClBr}$, *Phys. Rev. B* **112**, 134437 (2025).
- [18] I. S. Jacobs, J. W. Bray, H. R. Hart, L. V. Interrante, J. S. Kasper, G. D. Watkins, D. E. Prober, and J. C. Bonner, Spin-peierls transitions in magnetic donor-acceptor compounds of tetrathiafulvalene (TTF) with bisdithiolene metal complexes, *Phys. Rev. B* **14**, 3036 (1976).
- [19] M. Hase, I. Terasaki, and K. Uchinokura, Observation of the spin-peierls transition in linear Cu^{2+} (spin-1/2) chains in an inorganic compound CuGeO_3 , *Phys. Rev. Lett.* **70**, 3651 (1993).
- [20] S. K. Saha, M. S. Roy, M. Kumar, and Z. G. Soos, Modeling the spin-peierls transition of spin- $\frac{1}{2}$ chains with correlated states: $J_1 - J_2$ model, CuGeO_3 , and $\text{TTF} - \text{CuS}_4\text{C}_4(\text{CF}_3)_4$, *Phys. Rev. B* **101**, 054411 (2020).
- [21] B. Sriram Shastry and B. Sutherland, Exact ground state of a quantum mechanical antiferromagnet, *Physica B+C (Amsterdam)* **108**, 1069 (1981).
- [22] P. Corboz and F. Mila, Tensor network study of the Shastry-Sutherland model in zero magnetic field, *Phys. Rev. B* **87**, 115144 (2013).
- [23] H. Chen, G. Duan, C. Liu, Y. Cui, W. Yu, Z. Y. Xie, and R. Yu, Spin excitations of the Shastry–Sutherland model–altermagnetism and deconfined quantum criticality, *arXiv:2411.00301*.
- [24] L. L. Viteritti, R. Rende, A. Parola, S. Goldt, and F. Becca, Transformer wave function for two dimensional frustrated magnets: Emergence of a spin-liquid phase in the Shastry-Sutherland model, *Phys. Rev. B* **111**, 134411 (2025).
- [25] F. Ferrari and R. Valentí, Altermagnetism on the Shastry-Sutherland lattice, *Phys. Rev. B* **110**, 205140 (2024).
- [26] H. Menke, M. Klett, K. Kanoda, A. Georges, M. Ferrero, and T. Schäfer, Superconductivity and Mott physics in organic charge transfer materials, *Phys. Rev. Lett.* **133**, 136501 (2024).
- [27] J. Liebman, K. Miyagawa, K. Kanoda, and N. Drichko, Novel dipole-lattice coupling in the quantum spin liquid material $\kappa - (\text{BEDT} - \text{TTF})_2\text{Cu}_2(\text{CN})_3$, *Phys. Rev. B* **110**, 165105 (2024).
- [28] E. H. Lieb, M. Loss, and R. J. McCann, Uniform density theorem for the Hubbard model, *J. Math. Phys. (N.Y.)* **34**, 891 (1993).
- [29] K. Kubo and T. Kishi, Rigorous bounds on the susceptibilities of the Hubbard model, *Phys. Rev. B* **41**, 4866 (1990).
- [30] T. Koma and H. Tasaki, Decay of superconducting and magnetic correlations in one- and two-dimensional Hubbard models, *Phys. Rev. Lett.* **68**, 3248 (1992).
- [31] M. Yamanaka, M. Oshikawa, and I. Affleck, Nonperturbative approach to Luttinger’s theorem in one dimension, *Phys. Rev. Lett.* **79**, 1110 (1997).
- [32] M. Oshikawa, Commensurability, excitation gap, and topology in quantum many-particle systems on a periodic lattice, *Phys. Rev. Lett.* **84**, 1535 (2000).
- [33] H. Tasaki, The Hubbard model—an introduction and selected rigorous results, *J. Phys. Condens. Matter* **10**, 4353 (1998).
- [34] H. Tasaki, Half-filled models: Lieb’s theorems and the origin of antiferromagnetism and ferrimagnetism, in *Physics and Mathematics of Quantum Many-Body Systems* (Springer International Publishing, Cham, 2020), pp. 341–370, 10.1007/978-3-030-41265-4_10.
- [35] M. Qin, T. Schäfer, S. Andergassen, P. Corboz, and E. Gull, The Hubbard model: A computational perspective, *Annu. Rev. Condens. Matter Phys.* **13**, 275 (2022).

- [36] K. Kobayashi, M. Okumura, S. Yamada, M. Machida, and H. Aoki, Superconductivity in repulsively interacting fermions on a diamond chain: Flat-band-induced pairing, *Phys. Rev. B* **94**, 214501 (2016).
- [37] L. F. Tocchio, A. Montorsi, and F. Becca, Magnetic and spin-liquid phases in the frustrated $t - t'$ Hubbard model on the triangular lattice, *Phys. Rev. B* **102**, 115150 (2020).
- [38] C. Zhang, J.-W. Li, D. Nikolaidou, and J. von Delft, Frustration-induced superconductivity in the $t - t'$ Hubbard model, *Phys. Rev. Lett.* **134**, 116502 (2025).
- [39] D. P. Arovas, E. Berg, S. A. Kivelson, and S. Raghu, The Hubbard model, *Annu. Rev. Condens. Matter Phys.* **13**, 239 (2022).
- [40] R. Kuzian, Methods of modeling of strongly correlated electron systems, *Nanomaterials* **13**, 238 (2023).
- [41] H. C. Kandpal, I. Opahle, Y.-Z. Zhang, H. O. Jeschke, and R. Valentí, Revision of model parameters for κ -type charge transfer salts: An ab initio study, *Phys. Rev. Lett.* **103**, 067004 (2009).
- [42] B. Keimer, S. A. Kivelson, M. R. Norman, S. Uchida, and J. Zaanen, From quantum matter to high-temperature superconductivity in copper oxides, *Nature (London)* **518**, 179 (2015).
- [43] E. Dagotto, Correlated electrons in high-temperature superconductors, *Rev. Mod. Phys.* **66**, 763 (1994).
- [44] M. Danilov, E. G. C. P. van Loon, S. Brener, S. Isakov, M. I. Katsnelson, and A. I. Lichtenstein, Degenerate plaquette physics as key ingredient of high-temperature superconductivity in cuprates, *npj Quantum Mater.* **7**, 50 (2022).
- [45] M. Buzzi *et al.*, Photomolecular high-temperature superconductivity, *Phys. Rev. X* **10**, 031028 (2020).
- [46] J. Tindall, B. Buča, J. R. Coulthard, and D. Jaksch, Heating-induced long-range η pairing in the Hubbard model, *Phys. Rev. Lett.* **123**, 030603 (2019).
- [47] J. Tindall, F. Schlawin, M. A. Sentef, and D. Jaksch, Analytical solution for the steady states of the driven Hubbard model, *Phys. Rev. B* **103**, 035146 (2021).
- [48] J. Tindall, F. Schlawin, M. Sentef, and D. Jaksch, Lieb's theorem and maximum entropy condensates, *Quantum* **5**, 610 (2021).
- [49] J. Tindall, F. Schlawin, M. Buzzi, D. Nicoletti, J. R. Coulthard, H. Gao, A. Cavalleri, M. A. Sentef, and D. Jaksch, Dynamical order and superconductivity in a frustrated many-body system, *Phys. Rev. Lett.* **125**, 137001 (2020).
- [50] M. Buzzi, D. Nicoletti, S. Fava, G. Jotzu, K. Miyagawa, K. Kanoda, A. Henderson, T. Siegrist, J. A. Schlueter, M.-S. Nam, A. Ardavan, and A. Cavalleri, Phase diagram for light-induced superconductivity in $\kappa - (\text{ET})_2 - \text{X}$, *Phys. Rev. Lett.* **127**, 197002 (2021).
- [51] M. Iraola, N. Heinsdorf, A. Tiwari, D. Lessnich, T. Mertz, F. Ferrari, M. H. Fischer, S. M. Winter, F. Pollmann, T. Neupert, R. Valentí, and M. G. Vergniory, Towards a topological quantum chemistry description of correlated systems: The case of the Hubbard diamond chain, *Phys. Rev. B* **104**, 195125 (2021).
- [52] H. Pan, F. Wu, and S. Das Sarma, Band topology, Hubbard model, Heisenberg model, and dzyaloshinskii-moriya interaction in twisted bilayer wse_2 , *Phys. Rev. Res.* **2**, 033087 (2020).
- [53] T. Watanabe, H. Yokoyama, Y. Tanaka, and J. Inoue, Predominant magnetic states in the Hubbard model on anisotropic triangular lattices, *Phys. Rev. B* **77**, 214505 (2008).
- [54] R. T. Clay, H. Li, and S. Mazumdar, Absence of superconductivity in the half-filled band Hubbard model on the anisotropic triangular lattice, *Phys. Rev. Lett.* **101**, 166403 (2008).
- [55] T. Yoshioka, A. Koga, and N. Kawakami, Quantum phase transitions in the Hubbard model on a triangular lattice, *Phys. Rev. Lett.* **103**, 036401 (2009).
- [56] H.-Y. Yang, A. M. Läuchli, F. Mila, and K. P. Schmidt, Effective spin model for the spin-liquid phase of the Hubbard model on the triangular lattice, *Phys. Rev. Lett.* **105**, 267204 (2010).
- [57] H.-P. Cheng, S. Liu, X. Chen, L. Zhang, and J. N. Fry, First-principles study of magnetism and electric field effects in 2D systems, *AVS Quantum Sci.* **2**, 027101 (2020).
- [58] E. H. Lieb, Two theorems on the Hubbard model, *Phys. Rev. Lett.* **62**, 1201 (1989).
- [59] S.-Q. Shen, Z.-M. Qiu, and G.-S. Tian, Ferrimagnetic long-range order of the Hubbard model, *Phys. Rev. Lett.* **72**, 1280 (1994).
- [60] H. Tasaki, Extension of nagaoka's theorem on the large- u Hubbard model, *Phys. Rev. B* **40**, 9192 (1989).
- [61] A. Mielke, Ferromagnetism in the Hubbard model on line graphs and further considerations, *J. Phys. A* **24**, 3311 (1991).
- [62] A. Mielke, Stability of ferromagnetism in Hubbard models with degenerate single-particle ground states, *J. Phys. A* **32**, 8411 (1999).
- [63] A. Mielke, Ferromagnetism in single-band Hubbard models with a partially flat band, *Phys. Rev. Lett.* **82**, 4312 (1999).
- [64] A. Mielke, Properties of Hubbard models with degenerate localised single-particle eigenstates, *Eur. Phys. J. B* **85**, 184 (2012).
- [65] K.-S. Kim, Exact hole-induced resonating-valence-bond ground state in certain $U = \infty$ Hubbard models, *Phys. Rev. B* **107**, L140401 (2023).
- [66] K.-S. Kim and H. Katsura, Exact hole-induced $SU(N)$ flavor singlets in certain $U = \infty$ $SU(N)$ Hubbard models, *Phys. Rev. Res.* **6**, 013307 (2024).
- [67] C. Lacroix, P. Mendels, and F. Mila, *Introduction to Frustrated Magnetism*, 1st ed., Springer Series in Solid-State Sciences Vol. 164 (Springer, Berlin, Heidelberg, 2011), pp. XXVI–682, 10.1007/978-3-642-10589-0.
- [68] B. Sutherland and B. S. Shastry, Exact solution of a large class of interacting quantum systems exhibiting ground state singularities, *J. Stat. Phys.* **33**, 477 (1983).
- [69] M. W. Long and R. Fehrenbacher, An exactly soluble one-dimensional quantum mechanical Heisenberg and Nagaoka t - J model, *J. Phys. Condens. Matter* **2**, 2787 (1990).
- [70] K. Takano, K. Kubo, and H. Sakamoto, Ground states with cluster structures in a frustrated Heisenberg chain, *J. Phys. Condens. Matter* **8**, 6405 (1996).
- [71] J. Strečka, T. Verkholyak, J. Richter, K. Karl'ová, O. Derzhko, and J. Schnack, Frustrated magnetism of spin- $\frac{1}{2}$ Heisenberg diamond and octahedral chains as a statistical

- mechanical monomer-dimer problem, *Phys. Rev. B* **105**, 064420 (2022).
- [72] Y. Hirose, A. Oguchi, and Y. Fukumoto, Quantum dimer model containing Rokhsar-Kivelson point expressed by spin- $\frac{1}{2}$ Heisenberg antiferromagnets, *Phys. Rev. B* **101**, 174440 (2020).
- [73] J. Strečka, K. Karl'ová, T. Verkholyak, N. Caci, S. Wessel, and A. Honecker, Thermal first-order phase transitions, Ising critical points, and reentrance in the Ising-Heisenberg model on the diamond-decorated square lattice in a magnetic field, *Phys. Rev. B* **107**, 134402 (2023).
- [74] N. Caci, K. Karl'ová, T. Verkholyak, J. Strečka, S. Wessel, and A. Honecker, Phases of the spin- $\frac{1}{2}$ Heisenberg antiferromagnet on the diamond-decorated square lattice in a magnetic field, *Phys. Rev. B* **107**, 115143 (2023).
- [75] K. Karl'ová, A. Honecker, N. Caci, S. Wessel, J. Strečka, and T. Verkholyak, Thermodynamic properties of the macroscopically degenerate tetramer-dimer phase of the spin- $\frac{1}{2}$ Heisenberg model on the diamond-decorated square lattice, *Phys. Rev. B* **110**, 214429 (2024).
- [76] F. Gerken, I. Runkel, C. Schweigert, and T. Posske, All product eigenstates in Heisenberg models from a graphical construction, *Phys. Rev. Res.* **7**, L012008 (2025).
- [77] H. Jeschke, I. Opahle, H. Kandpal, R. Valentí, H. Das, T. Saha-Dasgupta, O. Janson, H. Rosner, A. Brühl, B. Wolf, M. Lang, J. Richter, S. Hu, X. Wang, R. Peters, T. Pruschke, and A. Honecker, Multistep approach to microscopic models for frustrated quantum magnets: The case of the natural mineral azurite, *Phys. Rev. Lett.* **106**, 217201 (2011).
- [78] M. Fujihala, H. Koorikawa, S. Mitsuda, K. Morita, T. Tohyama, K. Tomiyasu, A. Koda, H. Okabe, S. Itoh, T. Yokoo, S. Ibuka, M. Tadokoro, M. Itoh, H. Sagayama, R. Kumai, and Y. Murakami, Possible Tomonaga-Luttinger spin liquid state in the spin-1/2 inequilateral diamond-chain compound $K_3\text{Cu}_3\text{AlO}_2(\text{SO}_4)_4$, *Sci. Rep.* **7**, 16785 (2017).
- [79] M. Cui, N. Wang, S. Zhang, and Z. He, $\text{Cu}_3(\text{CH}_3\text{COO})_4(\text{OH})_2 \cdot 5\text{H}_2\text{O}$: A novel isolated spin-1/2 diamond chain compound showing possible valence-bond condensation, *Cryst. Growth Design* **19**, 547 (2019).
- [80] F. H. L. Essler, H. Frahm, F. Göhmann, A. Klümper, and V. E. Korepin, *The One-Dimensional Hubbard Model* (Cambridge University Press, Cambridge, England, 2005), 10.1017/CBO9780511534843.
- [81] A. H. MacDonald, S. M. Girvin, and D. Yoshioka, (t/U) expansion for the Hubbard model, *Phys. Rev. B* **37**, 9753 (1988).
- [82] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/wqw-3cbl> for magnetization of electronic ground states in frustrated superstable graphs.
- [83] A graph is connected if every element in v can be reached by traversing edges in e starting at any vertex in v .
- [84] E. Lieb and D. Mattis, Ordering energy levels of interacting spin systems, *J. Math. Phys. (N.Y.)* **3**, 749 (1962).
- [85] G.-S. Tian, Coexistence of the ferromagnetic and antiferromagnetic long-range orders in the generalized antiferromagnetic Heisenberg model on a bipartite lattice, *J. Phys. A* **27**, 2305 (1994).
- [86] F. Battiston, G. Cencetti, I. Iacopini, V. Latora, M. Lucas, A. Patania, J.-G. Young, and G. Petri, Networks beyond pairwise interactions: Structure and dynamics, *Phys. Rep.* **874**, 1 (2020).
- [87] R. M. McConnell and J. P. Spinrad, Modular decomposition and transitive orientation, *Discrete Math.* **201**, 189 (1999).
- [88] M. Habib and C. Paul, A survey of the algorithmic aspects of modular decomposition, *Comput. Sci. Rev.* **4**, 41 (2010).
- [89] A connected component is a subset of vertices in v such that every vertex in the subset can be reached from any other by traversing edges in e , and no additional vertices from v can be included without violating this property.
- [90] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, Commentary: The materials project: A materials genome approach to accelerating materials innovation, *APL Mater.* **1**, 011002 (2013).
- [91] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states, *Ann. Phys. (Amsterdam)* **326**, 96 (2011).
- [92] R. Orús, Tensor networks for complex quantum systems, *Nat. Rev. Phys.* **1**, 538 (2019).
- [93] M. Born and V. Fock, Beweis des adiabatensatzes, *Z. Phys.* **51**, 165 (1928).
- [94] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, England, 2000), 10.1017/CBO9780511622540.
- [95] M. Campostrini, J. Nespolo, A. Pelissetto, and E. Vicari, Finite-size scaling at first-order quantum transitions, *Phys. Rev. Lett.* **113**, 070402 (2014).
- [96] S. Hayami and Y. Motome, Topological spin crystals by itinerant frustration, *J. Phys. Condens. Matter* **33**, 443001 (2021).
- [97] M. Tepie, F. Glerean, J. Ovčar, S. Priya, K. Miyagawa, H. Taniguchi, K. Kanoda, I. Lončarić, M. Dressel, and M. Mitrano, Photoinduced frustration modulation in κ -type quantum spin liquid candidates, *Phys. Rev. B* **112**, L140401 (2025).
- [98] A. de la Torre, D. M. Kennes, M. Claassen, S. Gerber, J. W. McIver, and M. A. Sentef, Colloquium: Nonthermal pathways to ultrafast control in quantum materials, *Rev. Mod. Phys.* **93**, 041002 (2021).
- [99] J. Hauschild and F. Pollmann, Efficient numerical simulations with tensor networks: Tensor network python (tenpy), *SciPost Phys. Lect. Notes* **5** (2018).
- [100] S. Bravyi, D. P. DiVincenzo, and D. Loss, Schrieffer-Wolff transformation for quantum many-body systems, *Ann. Phys. (Amsterdam)* **326**, 2793 (2011).
- [101] T. Kato, *Perturbation Theory for Linear Operators*, 2nd ed., Classics in Mathematics (Springer, Berlin Heidelberg, 1995), 10.1007/978-3-642-66282-9.
- [102] R. Diestel, *Graph Theory*, 6th ed., Graduate Texts in Mathematics Vol. XX (Springer, Berlin, Heidelberg, 2025), p. 455, 10.1007/978-3-662-70107-2.

End Matter

The strongly correlated regime—

Definition 1 (Strongly correlated regime)—The strongly correlated regime is where U is sufficiently large so that the quantum number S can be continued to the S of a unique ground state predicted by the order n expansion in t/U of a Schrieffer-Wolff transformation.

This regime exists since, for sufficiently large U , the SW transformation expansion series is absolutely convergent (see Refs. [82,100]) and the ground state predicted from the order n expansion is robust to higher order terms [34,100,101].

Effective spin Hamiltonian of a superstable graph—A superstable graph yields, at some order n in the SW transformation expansion and up to a scale factor, an effective spin Hamiltonian of the form

$$H^{\text{SS}}(\beta) = H_{\text{H}}(G^{\text{C}}) + H_{\text{H}}(G_{\beta}^{\text{R}}) + \sum_{i=1}^{(n+1)/2} \sum_{q=1}^{Q_i} \beta^i \mathcal{X}_{i,q} \mathcal{Y}_{i,q}, \quad (\text{B1})$$

where the graphs G^{C} and G_{β}^{R} must be unions of connected bipartite graphs. Each connected component of G^{C} must be balanced, while at most one of the connected components of G_{β}^{R} can be unbalanced. Although G_{β}^{R} depends on $\beta > 0$, this parameter only rescales the weights without changing the vertex or the edge sets. The third term encodes the frustration in the system. The $\mathcal{X}_{i,q}$ ($\mathcal{Y}_{i,q}$) operators act on the subspace defined by the vertices of G^{C} (G_{β}^{R}). The total number of interactions for a given order i is Q_i , which depends on the edges connecting the components of G^{C} and G_{β}^{R} . To ensure the frustrating terms vanish, we require that the ground state of $H_{\text{H}}(G^{\text{C}})$ is superstable to all $\mathcal{X}_{i,q}$. Formally, this means the ground state of $H_{\text{H}}(G^{\text{C}})$ is an eigenstate of the operators $\mathcal{X}_{i,q}$ with eigenvalue 0 [68]. Consequently, the latter property enforces that the ground states of $H_{\text{H}}(G^{\text{C}}) + H_{\text{H}}(G_{\beta}^{\text{R}})$ are superstable to the frustrating term in Eq. (B1).

Algorithm to identify superstable graphs—We describe a constructive algorithm that, given an input graph G [cf. Fig. 2(a)], identifies features that lead to a Hamiltonian of the form of Eq. (B1). It relies on the identification of substructures of the graph, which we call cores. These structures are characterized through induced subgraphs [102]: we denote an induced subgraph of G as $G[M] = (M, E^M, t(E^M))$, where $G[M]$ takes all the edges and weights of G where both ends are elements of $M \subseteq V$. With this, we formally define.

Definition 2 (Core)—A subset $X \subseteq V$ is a core if the following conditions hold: 1. The induced subgraph $G[X]$ is

connected and balanced. 2. One of the following holds for each $v \in V \setminus X$: (i) v is not part of another core, and the weights from v to all vertices in X are equal, denoted by $t_X(v)$. That is, $t(v, x) = t_X(v) \forall x \in X$. (ii) v belongs to another core X' , and the weights connecting X and X' satisfy the relation $[t(x, v)]^2 = [t_{X-X'}(x)]^2 + [t_{X'-X}(v)]^2 \forall x \in X$ and $\forall v \in X'$. Here, $t_{X-X'}(x)$ represents a fixed weight contribution that depends on the module pair (X, X') but not on the specific vertex $v \in X'$. Similarly, $t_{X'-X}(v)$ represents the contribution that depends on v , but is independent of the specific $x \in X$.

The function $t_{X-X'}(x)$ captures how the weights connecting X to X' depend on the choice of vertex in X , but remain independent of the specific vertex in X' . This structure ensures that part of the weights connecting the two cores are uniform across all vertices in X' , guaranteeing superstability [82]. Similarly, the function $[t_{X'-X}(v)]$ ensures uniform connections between each vertex in X' and all the vertices in X . With the definition, we describe the algorithm below.

First, identify the presence of cores in the input graph and denote them as sets C_u , where $u \in \mathcal{I}_{\text{C}}$ with $\mathcal{I}_{\text{C}}$ the index set labeling the cores. This can be achieved through a generalized modular-decomposition algorithm [87,88] in which the usual definition of a module is supplemented by condition 1 and condition 2(ii) of Definition 2. After identifying the cores, define the residue $V^{\text{R}} := V \setminus \bigcup_{u \in \mathcal{I}_{\text{C}}} C_u$ [see Fig. 2(b)]. This yields the partition

$$G = \left(\bigoplus_{u \in \mathcal{I}_{\text{C}}} G[C_u] \right) \oplus G[V^{\text{R}}] \oplus \left(\emptyset, E^{\text{F}}, t(E^{\text{F}}) \right), \quad (\text{C1})$$

where $\oplus$ denotes the disjoint union of graph elements, and the set of edges $E^{\text{F}} := E \setminus [(\bigcup_{u \in \mathcal{I}_{\text{C}}} E^{C_u}) \cup E^{\text{R}}]$ are those generating frustration between cores or cores and residue.

Then verify whether $G[V^{\text{R}}]$ is bipartite with at most one unbalanced connected component. In that case, G is superstable and $n = 1$ is the order of the SW transformation expansion that leads to Eq. (B1) [82]. Then, $\bigoplus_{u \in \mathcal{I}_{\text{C}}} G[C_u] \equiv_{t(e) \neq 0} G^{\text{C}}$ and $G[V^{\text{R}}] \equiv_{t(e) \neq 0} G_{\beta}^{\text{R}}$, where $\equiv_{t(e) \neq 0}$ denotes equality up to weight magnitude: the vertex and edge sets coincide, but the actual weight values may differ.

If $G[V^{\text{R}}]$ is only bipartite, higher orders in the expansion may lead to Eq. (B1). In that case, check the following additional conditions that yield Eq. (B1) for the $n = 3$ expansion order [82]: (i) none of the connected components of $G[V^{\text{R}}]$ or $G[C_u]$ can have more than two vertices; (ii) the weights coupling different cores have to follow the additional constraint $t(x, v) = t_X(v) = t_{X'}(x) = t_{X-X'} = t_{X'-X}$ for $x \in X$, $v \in X'$, with $X \neq X'$; (iii) the $n = 3$ SW transformation expansion adds edges with ends in V^{R} that turn the effective spin model version of the subgraph $G[V^{\text{R}}]$ into G_{β}^{R} , which is a bipartite graph with at most one unbalanced component. These added edges depend on the walks

(routes following adjacent vertices) of the graph G involving edges in E^F . Only simple two paths and four cycles contribute to the $n = 3$ expansion order. Let $i, j, k, l \in V$ be distinct vertices. A simple two path consists of edges (i, j) and (j, k) . A four cycle is a set of four edges $(i, j), (j, k), (k, l), (l, i)$. The $n = 3$ expansion adds an edge between a pair of V^R vertices for each two path or four cycle that is formed exclusively from edges in E^F [cf. purple edge in Fig. 2(c)]. If, when added to $G[V^R]$, these new edges generate a bipartite graph, the input graph is superstable and we can determine the magnetic properties from the bipartition of the different $G[C_u]$, and $G[V^R]$ with the added edges [cf. Fig. 2(d)].

Proof of Theorem 1—Consider the Hamiltonian in Eq. (B1) and let $G^C = \bigoplus_{u \in \mathcal{I}} G^C[C_u]$ and $G_\beta^R = \bigoplus_{v \in \mathcal{I}} G_\beta^R[R_v]$. The set $\mathcal{I}$ is the index set labeling the components of the corresponding subgraphs. The $C_u \subseteq V^C$ ($R_v \subseteq V^R$) are such that $V^C = \bigsqcup_{u \in \mathcal{I}} C_u$ ($V^R = \bigsqcup_{v \in \mathcal{I}} R_v$). We construct a basis given by states $|j, k, \beta\rangle := |j\rangle_C \otimes |k, \beta\rangle_R$. Here, $|j\rangle_C$ are all the eigenstates of $H_H(G^C)$ with eigenvalue λ_j^C with $j \in [0, 2^{|V^C|} - 1] \subset \mathbb{N}$ ordered with increasing energy. According to the Lieb-Mattis theorem and the fact that the components of G^C are balanced, $|0\rangle_C$ is the unique ground state of $H_H(G^C)$ with $S = 0$ and we can define the energy gap $\Delta^C := \lambda_1^C - \lambda_0^C > 0$. Similarly, $|k, \beta\rangle_R$ are the eigenstates with energy $\lambda_k^R(\beta)$ of $H_H(G_\beta^R)$ with $k \in [0, 2^{|V^R|} - 1] \subset \mathbb{N}$. The unbalanced component of G_β^R implies the ground states of the Hamiltonian $H_H(G_\beta^R)$ have an S given by Theorem 1. Therefore, the ground states have energy $\lambda_0^R(\beta) = \lambda_m^R(\beta) \forall m \in [0, 2S] \subset \mathbb{N}$ and we can define the gap $\Delta^R(\beta) := \lambda_{2S+1}^R(\beta) - \lambda_0^R(\beta)$.

Now, we assume that $|0\rangle_C$ is superstable with respect to all $\mathcal{X}_{i,q}$. It implies $|0, k, \beta\rangle$ is superstable to the interactions in Eq. (B1) $\forall k, \beta$. Consider the subset of superstable states given by $|0, m, \beta\rangle$ with m in the abovementioned range. We want to show that there exists a range of positive β such that the $|0, m, \beta\rangle$ are the only ground states for Eq. (B1) and that these are gapped from the rest of the spectrum. These states have a total spin S as defined in Theorem 1, respecting the trivial degeneracy.

The states $|0, m, \beta\rangle$ have eigenvalues $E_0^{\text{SS}}(\beta) := \lambda_0^C + \lambda_0^R(\beta)$, and we require $E_0^{\text{SS}}(\beta) < \langle \psi | H^{\text{SS}}(\beta) | \psi \rangle$ for all other eigenstates of $H^{\text{SS}}(\beta)$. We start by comparing the other superstable states $|0, k > 2S, \beta\rangle$. Their energy is bounded from below as

$$\langle 0, k > 2S, \beta | H^{\text{SS}}(\beta) | 0, k > 2S, \beta \rangle \geq E_0^{\text{SS}}(\beta) + \Delta^R(\beta).$$

This lower bound is always larger than $E_0^{\text{SS}}(\beta)$. Hence, none of the other superstable states can feature equal or

lower eigenenergies than $E_0^{\text{SS}}(\beta)$. All the other eigenstates orthogonal to $|0, k, \beta\rangle \forall k$ may be expanded as

$$|\psi\rangle = \sum_{j=1}^{2^{|V^C|}-1} \sum_{k=0}^{2^{|V^R|}-1} C_{j,k} |j, k, \beta\rangle.$$

It is easy to show that any state of this form provides a lower bound for the energy as

$$\langle \psi | H^{\text{SS}}(\beta) | \psi \rangle \geq E_0^{\text{SS}}(\beta) + \Delta^C - \sum_{i=1}^{(n+1)/2} \beta^i \bar{Q} \bar{\mathcal{X}} \bar{\mathcal{Y}},$$

where $\bar{Q} := \max_i(Q_i)$, $\bar{\mathcal{X}} := \max_{i,q}(\|\mathcal{X}_{i,q}\|)$, and $\bar{\mathcal{Y}} := \max_{i,q}(\|\mathcal{Y}_{i,q}\|)$; with $\|O\|$ denoting the operator norm of the operator O . Consequently,

$$\beta \frac{1 - \beta^{(n+1)/2}}{1 - \beta} \bar{Q} \bar{\mathcal{X}} \bar{\mathcal{Y}} < \Delta^C \quad (\text{C2})$$

provides a sufficient condition so that $|0, m, \beta\rangle$ are the gapped ground states for finite β . In other words, this inequality determines the regime of sufficiently small β where the ground states are only the superstable states $|0, m, \beta\rangle$.

Therefore, for sufficiently small β , the ground states of a Hamiltonian proportional to Eq. (B1) are exactly $(2S + 1)$ degenerate, each being the unique ground state with a different quantum number for the spin projection along the z -axis. Any ground state that can be adiabatically continued to one of these while preserving the $\text{SU}(2)$ symmetry must have the same total spin quantum number S . This establishes that the ground state of the Hubbard model on a superstable graph has total spin given by S in the strongly correlated regime for sufficiently small β . ■

Proof of Corollary 1—For sufficiently large U and sufficiently small β , the ground states of the Hamiltonian obtained by the order n expansion are given by

$$|0, m, \beta\rangle = \bigotimes_{u \in \mathcal{I}} |0\rangle_{C_u} \bigotimes_{v \in \mathcal{I}; v \neq 0} |0, \beta\rangle_{R_v} \otimes |m, \beta\rangle_{R_0}, \quad (\text{C3})$$

with $|0\rangle_{C_u}$ the ground state of $H_H(G^C[C_u])$. Here, $|k, \beta\rangle_{R_v}$ is the k th eigenvector ordered ascendingly in the eigenvalues of $H_H(G_\beta^R[R_v])$ and R_0 is the set of vertices corresponding to the only unbalanced component of G_β^R . This product form of the wave function ensures the correlations between the spaces spanned by the different components vanish. Within each component of $G^C \oplus G_\beta^R$, the Shen-Qiu-Tian theorem gives the sign of the ground state correlations of the effective model. As shown in [82], the $\langle S_i^+ S_j^- \rangle$ correlations of the effective model obtained through the SW transformation represent the correlations of the original system up to $O(U^{-2})$ corrections. ■