

Breakdown of the Thermodynamic Limit in Quantum Spin and Dimer Models

Jeet Shah^{1,2,*}, Laura Shou^{1,*}, Jeremy Shuler¹, and Victor Galitski¹

¹*Joint Quantum Institute, Department of Physics, University of Maryland,
College Park, Maryland 20742, USA*

²*Joint Center for Quantum Information and Computer Science, NIST/University of Maryland,
College Park, Maryland 20742, USA*



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The thermodynamic limit is foundational to statistical mechanics, underlying our understanding of many-body phases. It assumes that, as the system size grows infinitely at fixed density of particles, unambiguous macroscopic phases emerge that are independent of the system's boundary shape. We present explicit quantum spin and dimer Hamiltonians whose ground states violate this principle. Our construction relies on the previous mathematical work on classical dimers on the Aztec diamond and the square-octagon fortress, where geometry-dependent phase behaviors are observed in the infinite-size limit. We reverse engineer quantum spin Hamiltonians on the square and the square-octagon lattices whose ground states at the Rokhsar-Kivelson points are described by classical dimer coverings. On diamond-shaped domains, we find macroscopic boundary regions exhibiting distinct quantum phases from those on square-shaped domains. We study the nature of these phases by calculating the dimer-dimer and vison correlators and adapt Kasteleyn matrix based analytical and numerical methods for computing the vison correlator, which are significantly more efficient than standard Monte Carlo techniques. Our results show that the square-octagon lattice supports a single gapped short-range entangled phase, with exponentially decaying dimer correlators and a constant vison correlator. When the same model is considered on a diamond-shaped domain, two additional macroscopic regions emerge, with one near the corners and exhibiting staggered dimer order, and another exhibiting critical correlations.

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I. INTRODUCTION

A foundational assumption of statistical mechanics is that, in the thermodynamic limit, the shape of the system's boundary does not influence its bulk properties. This is consistent with everyday experience: a cubic piece of iron is metallic throughout the bulk, as is a spherical piece of iron. The negligible influence of the boundaries allows us to define a macroscopic bulk phase with uniform properties throughout and choose boundary conditions as convenient. For a single particle, boundary sensitivity is familiar: the choice of boundary conditions and geometry directly quantizes the allowed wave functions and spectra. In contrast, for generic interacting many-body systems with local interactions, boundary effects are expected to be

confined to a thin edge region, so bulk observables become independent of boundary shape in the thermodynamic limit. Here we generalize this notion by showing that the boundary *shape* can instead induce macroscopic regions with different bulk phases, so local correlators deep in the interior remain boundary dependent even as the system size tends to infinity.

In this work, we present two quantum spin models with local interactions that map to quantum dimer models, for which this assumption fails—i.e., the thermodynamic limit breaks down, and the shape of the system boundaries have a profound effect on the bulk phases. Dimers are degrees of freedom that occupy pairs of neighboring sites, with the constraint that no two dimers share a site. In the context of graph theory, dimer coverings are known as perfect matchings. Quantum dimer models were first introduced by Rokhsar and Kivelson in Ref. [1], where they studied such a model on the square lattice. Their Hamiltonian consisted of off-diagonal ring-exchange terms and diagonal Rokhsar-Kivelson (RK) potential energy terms. At the RK point, where these terms have equal strength, the ground state is exactly solvable, and the dimer-dimer connected

*These authors contributed equally to this work.

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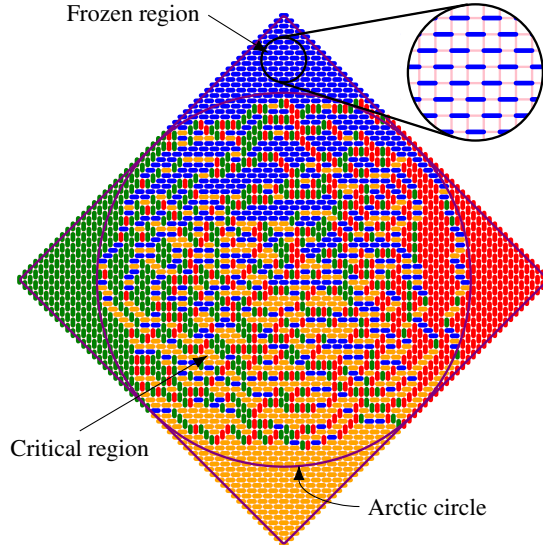


FIG. 1. A random dimer covering of an Aztec diamond, generated via Monte Carlo simulation. The Aztec diamond is a bipartite graph, with vertices partitioned into two sublattices—commonly referred to as “black” and “white” vertices. Red and green edges represent vertical dimers, while blue and orange edges represent horizontal dimers; the two colors for each orientation indicate whether the black vertex lies on the top or bottom (for vertical) or left or right (for horizontal) end of the dimer. The purple circle indicates the *Arctic circle*. Outside the Arctic circle, the system is *frozen*—dimers align in a staggered configuration (as shown in the inset) with probability tending to one as the diamond size tends to infinity. Inside the Arctic circle, dimers can have random orientations. This configuration was generated by starting from an initial configuration with all horizontal dimers and performing 10^{11} ring-flip moves.

correlator exhibits power-law decay, implying that the model is at a critical point in the phase diagram. Remarkably, we find that for the same quantum dimer model when considered on the square lattice with boundaries at $\pm 45^\circ$ to the edges, different regions in the bulk have drastically different behavior. Such a square lattice with diamond shaped ($\diamond$) boundaries is called the “Aztec diamond” [2]. Figure 1 shows an Aztec diamond along with one of its dimer coverings chosen randomly from the set of all dimer coverings. This model is our first example of the breakdown of the thermodynamic limit. One can immediately see phase separation in this figure: regions near the corners display a staggered dimer configuration, while the dimers within a circle inscribed in the diamond, known as the “Arctic circle” [3], exhibit no apparent order. This phenomenon in uniformly sampled random dimer coverings of the Aztec diamond is well known in the mathematical literature as the “Arctic circle theorem” [2–8], and was proved by Jockusch, Propp, and Shor in Ref. [3]. The Arctic circle phenomenon implies that for the RK dimer model on the Aztec diamond, the corners are in a *frozen* phase, while the region inside the Arctic circle will be critical, having power-law decaying dimer correlations.

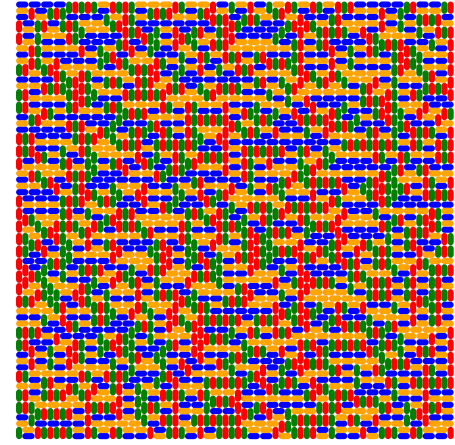


FIG. 2. A random dimer configuration on the square lattice with square-shaped boundaries, generated via Monte Carlo sampling. Different colors indicate dimer orientations.

This provides a rigorous example of spatial separation between quantum phases induced by the shape of the boundary. Notably, the frozen regions are macroscopic relative to the system as a whole, implying that the phase separation is not localized to the boundaries. In contrast, the quantum dimer model on the square lattice with rectangular boundaries, as proposed by Rokhsar and Kivelson in Ref. [1], does not exhibit such a phase separation. Figure 2 shows a randomly chosen dimer configuration of the square lattice on a square-shaped domain, where it is apparent that no frozen regions appear. Importantly, we keep the bulk Hamiltonian the same for both the Aztec diamond and rectangular boundaries in the quantum dimer model. Because differently shaped pieces of the same model display drastically different bulk behavior, the thermodynamic limit is not well defined. As the system size tends to infinity, one must also specify the shape of the system and the location of the origin relative to that shape.

Boundary dependence on the phase of macroscopic regions of classical dimer models has been well-studied as noted earlier [8–10]. Such a boundary dependence has also been observed and studied in the context of classical six-vertex models in Refs. [11–15], which can be related to interacting classical dimer models [16]. In this paper, however, we are concerned with *quantum* models having such boundary dependence. In this context, we note that boundary dependence of the ground state entropy in a bilayer quantum Heisenberg antiferromagnet model was recently found in Ref. [17], using a mapping of the ground states to classical dimers on the hexagonal lattice. Although Ref. [17] did not investigate coexistence of distinct phases together in the same system, we anticipate that the quantum phase coexistence we find in this paper could also be relevant for further investigation of the boundary dependence on entropy observed in such models. Boundary sensitivity is also present in fracton topological orders associated with subsystem symmetries in $(3 + 1)D$, where

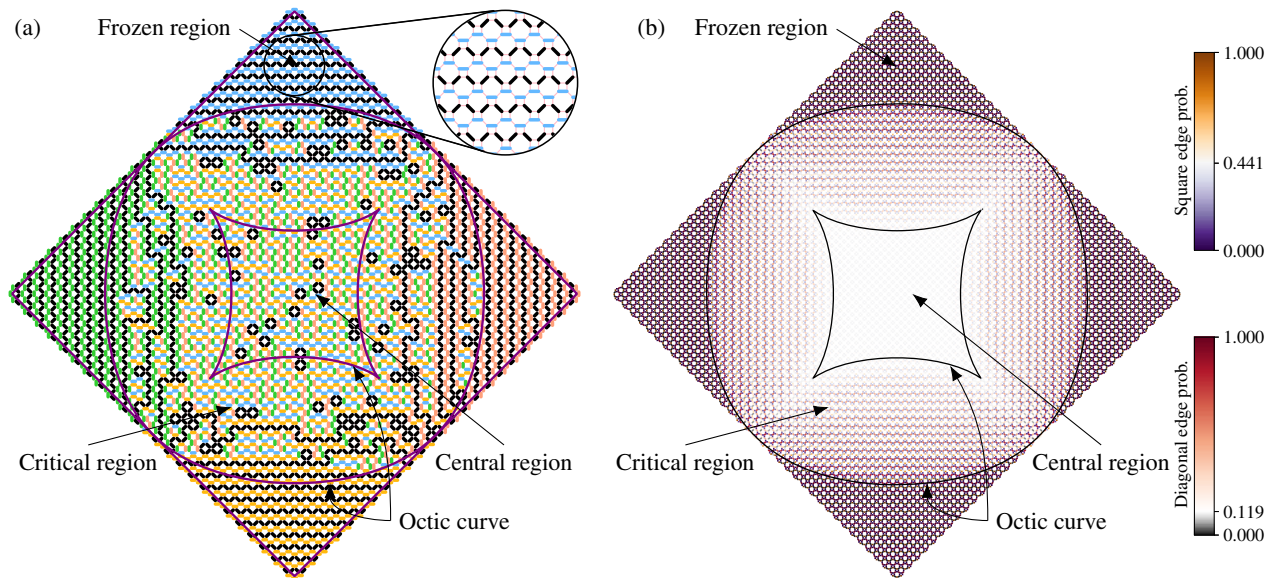


FIG. 3. (a) A random dimer covering of the square-octagon fortress, generated via Monte Carlo simulation. Edges colored in red, blue, green, and orange represent horizontal and vertical dimers, while black links represent diagonal dimers. The octic curve separates the graph into three distinct regions. The regions near the four corners are called the *frozen regions*, where dimers exhibit an ordered configuration as shown in the inset. The *critical region*, located between the oval and the star-shaped curves, shows power-law decay in the dimer-dimer connected correlator. The innermost *central region* features an exponentially decaying dimer-dimer connected correlator. (b) A color plot showing the probability with which dimers occupy each edge. The color scale is set such that white corresponds to a probability of 0.441 on horizontal and vertical edges, and 0.119 on diagonal edges. These values are the analytically calculated dimer probabilities for the infinite square-octagon lattice with square boundaries, as derived in Appendix B 3. The center region appears white, indicating probabilities close to the infinite-limit rectangular boundary values, while the frozen corner regions appear dark brown, purple, red, or black, indicating dimer probabilities close to zero or one. The critical region between the center and the frozen corners shows a mix of colors that vary with position. All probabilities are calculated using exact fraction-free LU decomposition, as described in Sec. II B.

bulk braiding of excitations could be sensitive to the geometry [18]. Such models are also known to have ground state degeneracies which depend on the system size, going against the standard notions of the thermodynamic limit [19,20].

Dimer models have long attracted interest from both physicists and mathematicians, albeit for different reasons. In physics, early work [21–24] studied the relationship between correlation functions in classical dimer models and those in Ising models. Since then, quantum dimer models have been studied because they can exhibit exotic states of matter such as topologically ordered quantum spin liquids which have fractionalized excitations [25–33].

In mathematics, the combinatorics of dimer coverings on the Aztec diamond were first studied in Ref. [2]. Since then, there has been much work on weighted dimer coverings of the Aztec diamond [34–41], where the probability of a dimer covering is proportional to the product of weights on edges occupied by dimers. For different weights, shapes, or (bipartite) lattices, it is well known that various different curves separating up to three distinct phases are possible [37,42]. Additionally, there are deep connections between weighted dimer models and algebraic geometry: for example, the curves separating distinct phases, the number of

“gaseous” phase regions, and the limiting shape behaviors in the model, all have geometric identifications with properties of Riemann surfaces [40,42].

Returning to the quantum dimer model on the Aztec diamond, we note that since the region inside the Arctic circle is a critical region, it is not guaranteed if the quantum phase separation only occurs at the fine-tuned RK point or is stable to perturbations. It is possible and likely that perturbations away from the RK point will drive the critical region into an ordered phase, resulting in a uniform phase without any phase separation. This raises a natural question: can the breakdown of the thermodynamic limit and the spatial separation of quantum phases persist over an extended region of the phase diagram? We show that this is likely possible by introducing our second model, defined on the square-octagon lattice (also known as the truncated square lattice) which consists of alternating squares and octagons. In Fig. 3(a), we show a random dimer covering on a diamond-shaped domain of the square-octagon lattice, known as the “square-octagon fortress.” From this figure, it is clear that, similar to the Aztec diamond, the corners of the square-octagon fortress exhibit an ordered dimer configuration [7]. The analog of the Arctic circle in this geometry is an octic curve [7,37] that is the union of the oval and the

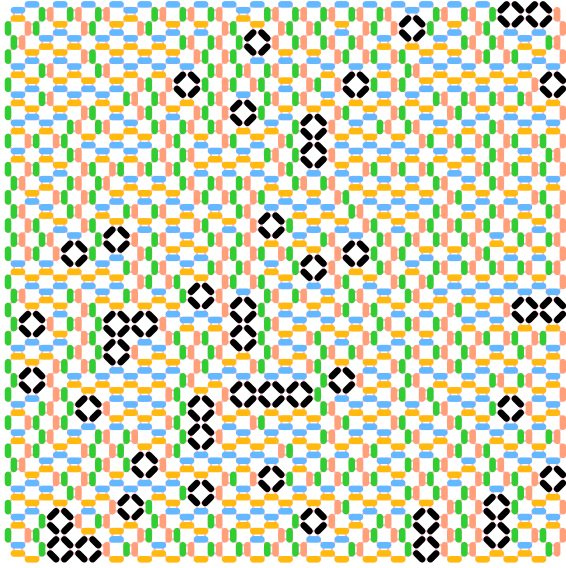


FIG. 4. A random dimer configuration of the square-octagon lattice with rectangular boundaries. Horizontal dimers are colored blue or orange, vertical dimers are colored green or pink, and diagonal dimers are colored black. We see that all diagonal dimers appear as a part of some flippable octagon. This phase can be viewed as a background of flippable square plaquettes, interspersed with a finite density of black flippable octagons.

star-shaped curves shown in Fig. 3. The “critical region” between these two curves is well expected to have dimer-dimer connected correlators with power-law decay, while in the innermost region these correlators are well expected to decay exponentially in the infinite-size limit, due to a relation with the dimer model on certain weighted Aztec diamonds [7,34,36,37]. We confirm the latter expectation numerically. Although these regions are shown for a single dimer covering in the figure, the ground state of our quantum spin and dimer models at the RK point, which are a superposition of exponentially many dimer coverings, also possess these three regions. These three regions are also clearly visible in the plot of dimer occupation probabilities for the RK wave function, shown in Fig. 3(b). In contrast, for the square-octagon lattice with square boundaries, a randomly sampled dimer covering has neither the frozen nor critical regions, as seen from a typical dimer covering displayed in Fig. 4. Perturbing away from the RK point of our dimer model, we expect the innermost region and the frozen corners with staggered order, to continue to exist. This expectation is based on these two regions being gapped which we conclude from the exponential decay of the dimer-dimer connected correlator. Since these are two different orders, we expect there to be an intermediate critical region across which the order changes. Thus, away from the RK point, we expect there to be two macroscopic ordered regions separated by an intermediate critical region. This demonstrates that the breakdown of the thermodynamic limit can persist beyond fine-tuned points and

remain robust to perturbations. We emphasize here that for a complete validation of this expectation of the phase separation away from the RK point, one would need to perform quantum Monte Carlo simulations, which we have left for a future work.

We also investigate the phases of our dimer models on the square-octagon lattice with both rectangular and square-octagon fortress boundaries at their respective RK points. Quantum dimer models are known to host exotic phases, such as quantum spin liquids—topologically ordered and highly entangled phases that are described by deconfined phases of gauge theories [28,43]. For example, the RK quantum dimer model on the triangular lattice is known to lie in a $\mathbb{Z}_2$ quantum spin liquid phase [30,44,45]. A $\mathbb{Z}_2$ quantum spin liquid phase supports two types of gapped excitations: electric charges and visons [29]. As a result, all correlators, including both the dimer-dimer connected correlator and the nonlocal vison correlator must decay exponentially with distance. The vison, defined using a string operator, is a topological excitation that is a relative semion with respect to the electric charge: braiding one around the other produces a statistical phase of -1 . The presence of gapped visons implies fractionalization, and thus the existence of a quantum spin liquid [29], since gapped visons are not present in the ground state, causing the electric charges to be deconfined [27]. Therefore, calculating the vison correlator is crucial for diagnosing if the dimer model is in a quantum spin liquid phase or not. While classical Monte Carlo methods are often used to estimate the vison correlators [27,45,46], they only provide approximate values due to finite sampling. In this work, we describe an exact method to calculate the vison correlator using the Kasteleyn matrix [21–23] and its inverse. This approach applies to the RK wave function on any planar lattice. This method allows us to calculate the vison correlator easily to arbitrary precision (here we go up to 10^{-21}), while Monte Carlo calculations would only give an accuracy of 10^{-6} in reasonable times. Furthermore, along certain paths of the square-octagon lattice with rectangular boundaries, we utilize the Toeplitz structure of the inverse Kasteleyn matrices to determine the vison correlator analytically.

We calculate the dimer-dimer connected and vison correlators in the central region of the square-octagon fortress, as well as in the square-octagon lattice with rectangular boundaries, to determine whether these regions realize a quantum spin liquid phase. In both geometries, we find that the dimer-dimer connected correlator decays exponentially, while the vison correlator approaches a constant along certain paths. Moreover, the asymptotic values of the vison correlators appear to be essentially the same in both cases. This rules out the possibility of a $\mathbb{Z}_2$ quantum spin liquid phase in these regions, indicating that the system is instead in an ordered phase. We identify the nature of the order by studying the conditional probabilities of diagonal dimers and conclude that the system is in a

short range entangled state similar to the Ruby family of Ref. [47].

The structure of the paper is as follows. In Sec. II, we begin by reviewing the Kasteleyn method to calculate the partition function and dimer probabilities. We then describe an exact method to calculate vison correlators for a general planar graph. Next, in Sec. III, we provide our first example of the breakdown of the thermodynamic limit on the Aztec diamond. We define a quantum spin Hamiltonian that maps to a quantum dimer model on both the square lattice with rectangular boundaries and the Aztec diamond. Section IV focuses on the square-octagon lattice with rectangular boundaries. We define the corresponding spin and low-energy effective dimer Hamiltonians and calculate dimer-dimer correlators in the infinite lattice limit using the asymptotic form of the Kasteleyn matrix inverse. Using the method of Sec. II B, we calculate the vison correlator and find that it approaches a constant along certain paths, implying that the system is in an ordered phase. We end the section by commenting on the nature of the ordered phase. In Sec. V, we provide our second example of the breakdown of the thermodynamic limit—this time likely stable to perturbations—by studying the quantum dimer model on the square-octagon fortress. We define the spin and dimer Hamiltonians as in the other sections, discuss the connection between the fortress and weighted Aztec diamonds, and calculate the dimer-dimer and vison correlators. We find that the central region behaves exactly like the square-octagon lattice with rectangular boundaries considered in Sec. IV. We again comment on the nature of the order in different regions. Finally, in Sec. VI, we summarize our results and outline several future directions.

II. EXACT CORRELATORS VIA KASTELEYN METHOD

In this section, we briefly review Kasteleyn's method for counting the total number of dimer coverings of a planar graph, and describe its standard application to calculating dimer-dimer correlators. For further references, see Kasteleyn's original papers [21,48,49] and the overviews in Refs. [8–10]. We then present an efficient, lesser-known method for calculating the vison correlator *exactly*, which will be useful for both numerical and analytical calculations in Secs. III to V.

A. Kasteleyn method overview

We start by counting the number of dimer coverings of a bipartite planar graph G with $2N$ vertices. A dimer covering, also known as a perfect matching of a graph, is a set of edges such that each vertex is connected to exactly one edge in the set. Since G is bipartite, we can color its vertices with two colors, say black and white, creating two disjoint sets $B = \{b_1, \dots, b_N\}$ and $W = \{w_1, \dots, w_N\}$, where a vertex $b \in B$ connects only to vertices $w \in W$, and vice

versa. Due to the bipartite structure, all graph information is captured in a reduced, half-size $N \times N$ adjacency matrix A , with rows indexed by vertices in B and columns indexed by vertices in W . This matrix is defined as $A(b_i, w_j) = 1$ if vertices $b_i \in B$ and $w_j \in W$ are connected by an edge, and 0 otherwise. The determinant of A expands as

$$\det A = \sum_{\sigma \in S_N} \text{sgn}(\sigma) A(b_1, w_{\sigma(1)}) \cdots A(b_N, w_{\sigma(N)}), \quad (1)$$

where S_N is the set of all permutations of N elements. From this expansion, we see that there is a bijection between the nonzero terms in the sum and the dimer coverings of G . However, this determinant need not count the total number of dimer coverings, due to the sign $\text{sgn}(\sigma)$ which can cause cancellations. For planar graphs, Kasteleyn [21,48] showed how to construct a *signed* adjacency matrix K , now called a Kasteleyn matrix, such that all nonzero terms in the sum for $\det K$ have the same sign. This gives the result

$$\text{Number of dimer coverings} = |\det K|. \quad (2)$$

The construction of a Kasteleyn matrix is always possible for planar graphs, and can be extended to count dimer coverings on a torus using four determinants [21] which we briefly review in Appendix A. The Kasteleyn matrix K is constructed from a *Kasteleyn orientation*, which for planar graphs is an assignment of directions to each edge such that every face has an odd number of edges oriented clockwise around its boundary [9,31,48,49]. For each directed edge $(b \rightarrow w)$, we assign it a positive (+1) orientation if it agrees with the Kasteleyn orientation and a negative (−1) orientation if it disagrees. An example Kasteleyn orientation for the square lattice is shown in Fig. 5. The Kasteleyn matrix K is then defined as

$$K(b, w) = \begin{cases} 1, & (b \rightarrow w) \text{ has positive orientation} \\ -1, & (b \rightarrow w) \text{ has negative orientation} \\ 0, & (b, w) \text{ is not an edge} \end{cases} \quad (3)$$

More generally, for nonbipartite graphs, one uses the same method but with a full-size $2N \times 2N$ Kasteleyn matrix $\mathbb{K}$

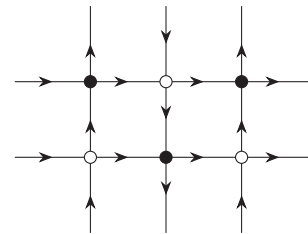


FIG. 5. A Kasteleyn orientation on the square lattice: all horizontal edges are oriented to the right, while vertical edges alternate in direction from column to column.

and its Pfaffian (see, e.g., [9,21] or Appendix B 1 for a brief review). However, since this paper focuses on the Aztec diamond and square-octagon graphs, which are bipartite, we will primarily work with the smaller, “half-size” Kasteleyn matrices K . We also note that nonplanar graphs can sometimes possess a Kasteleyn orientation. Precisely, a graph has a Kasteleyn orientation if and only if it does not have the utility graph $K_{3,3}$ as a minor [8,50,51]. Solvable nonplanar dimer models have been studied in, e.g., [24,52].

Kasteleyn’s method gives a formula for the probability that a particular set of dimers appear, expressed in terms of the inverse of the Kasteleyn matrix K . In the context of bipartite lattices, this is often referred to as Kenyon’s formula after Ref. [5]. The number of dimer coverings where a dimer occupies each edge in a set of edges E , can be counted using Kasteleyn’s method by noting that enforcing the presence of a dimer on an edge $e = (b, w)$ is effectively equivalent to removing the vertices b and w (along with all their incident edges) from the graph. This implies that the number of dimer coverings with dimers on all edges in E is given by the determinant of a submatrix of K , which, by Jacobi’s minor theorem, can be written in terms of the matrix elements of K and K^{-1} corresponding to the vertices in E .

Kenyon’s formula [5]. Let K be a Kasteleyn matrix for a bipartite graph G . Given a set of edges $E = \{e_1, \dots, e_k\}$, with $e_i = (b_i, w_i)$, the probability that the edges in E occur in a dimer covering is

$$\begin{aligned} & \mathbb{P}[e_1, \dots, e_k \text{ all occur in a dimer covering}] \\ &= \left[\prod_{i=1}^k K(b_i, w_i) \right] \det [K^{-1}(w_i, b_j)]_{1 \leq i, j \leq k}, \end{aligned} \quad (4)$$

where the determinant is over the submatrix of K^{-1} indexed by rows w_i and columns b_j , $(w_i, b_j)_{1 \leq i, j \leq k}$.

Kenyon’s formula is commonly used to calculate an important quantity—the dimer-dimer connected correlator, defined as

$$C_{\mu\nu}^d = \langle d_\mu d_\nu \rangle - \langle d_\mu \rangle \langle d_\nu \rangle, \quad (5)$$

where μ and ν label edges of the graph, and $d_\mu = 1$ if a dimer is present on edge μ , and $d_\mu = 0$ otherwise. Letting $\mu = (b_1, w_1)$ and $\nu = (b_2, w_2)$, Eq. (4) implies

$$C_{\mu\nu}^d = -K(b_1, w_1)K(b_2, w_2)K^{-1}(w_2, b_1)K^{-1}(w_1, b_2). \quad (6)$$

Therefore, knowing the values of K^{-1} on the relevant vertices allows one to calculate the dimer-dimer correlator. More generally, Eq. (4) shows that the matrix L defined by $L(w_i, b_j) = K(b_i, w_i)K^{-1}(w_i, b_j)$, serves as the correlation kernel for the determinantal point process formed by the edges [5,8].

B. Vison correlator via Kasteleyn matrices

In this section, we explain how to calculate the vison correlator both efficiently and exactly. It is well known that dimer models can be written as $\mathbb{Z}_2$ gauge theories [27,28,43]. The electric charges of these gauge theories correspond to sites where the dimer constraint is violated while the flux excitations of these theories are known as visons. The vison correlator [29,53,54] is a nonlocal string correlator that serves as a key diagnostic for identifying phases in quantum dimer models [55]. If the vison correlator decays exponentially with the distance between the string end points, the visons are gapped and can be viewed as excitations of the dimer model, implying the presence of fractionalized quasiparticles and that the system is a quantum spin liquid.

The type of calculation presented here traces back to the work of Onsager in the 1950s, Kasteleyn [21], and Montroll, Potts, and Ward [24] concerning spin correlations. However, in the context of visons, this method is often overlooked in favor of approximate approaches such as random sampling or Monte Carlo methods.

We focus on planar bipartite graphs with $2N$ vertices, where we can work with the half-size Kasteleyn matrices K , although the same method (using the full-size Kasteleyn matrices and Pfaffians) applies to nonbipartite planar graphs. The case of graphs on a torus is also similar; since we will use this for analytic results, we describe the necessary adjustments in Appendix A.

For a fixed path p between faces f_1 and f_2 , let $E = \{e_1, \dots, e_\ell\}$ be the set of edges crossed by p . Given a dimer configuration $\mathcal{C}$, let $\eta_E = \eta_E(\mathcal{C})$ denote the number of dimers present on the edges in E . The vison correlator between f_1 and f_2 —which is independent of the choice of path p as long as the paths are deformable into each other—is

$$\langle (-1)^{\eta_E} \rangle = \frac{\sum_{\{\text{configs. } \mathcal{C}\}} (-1)^{\eta_E(\mathcal{C})}}{\sum_{\{\text{configs. } \mathcal{C}\}} 1} = \frac{\det \tilde{K}}{\det K}, \quad (7)$$

where $\tilde{K}$ is defined as

$$\tilde{K}(b, w) = \begin{cases} -K(b, w), & (b, w) \text{ is an edge in } E \\ K(b, w), & \text{otherwise} \end{cases}. \quad (8)$$

The determinant $\det \tilde{K}$ counts the signed sum $\sum_{\{\text{configs. } \mathcal{C}\}} (-1)^{\eta_E(\mathcal{C})}$ for the same reason that $\det K$ counts the total number of configurations: the Kasteleyn orientation of K was chosen precisely so that every nonzero term $\text{sgn}(\sigma)K(b_1, w_{\sigma(1)}) \cdots K(b_N, w_{\sigma(N)})$ in the determinant expansion [cf. Eq. (1)] has the same sign. By flipping the sign in $\tilde{K}$ along every edge (b, w) in E , a given term $\text{sgn}(\sigma)\tilde{K}(b_1, w_{\sigma(1)}) \cdots \tilde{K}(b_N, w_{\sigma(N)})$ picks up an additional negative sign if and only if the configuration contains an odd number of dimers on edges in E . Thus, $\det \tilde{K}$ is equal

(up to an overall sign) to $\sum_{\{\text{configs. } C\}} (-1)^{\eta_E(C)}$. Equation (7) can be simplified further. Since $\tilde{K} = K - 2K'$, where

$$K'(b, w) = \begin{cases} K(b, w), & (b, w) \text{ is an edge in } E \\ 0, & \text{otherwise} \end{cases}, \quad (9)$$

we can view K' as a block matrix with only one nonzero block. This gives

$$\begin{aligned} \langle (-1)^{\eta_E} \rangle &= \frac{\det \tilde{K}}{\det K} = \det (I - 2K'K^{-1}) \\ &= \det (I_\ell - 2(K')_E(K^{-1})_E), \end{aligned} \quad (10)$$

where $(K^{-1})_E$ and $(K')_E$ are the submatrices corresponding to the vertices in E . Because this is only an $\ell \times \ell$ matrix determinant (for the bipartite case; in the nonbipartite case, it is the square root of a $2\ell \times 2\ell$ determinant), it becomes very convenient to calculate, provided we can reliably extract the required $\ell \times \ell$ submatrix of K^{-1} . In the case of an infinite periodic lattice (with periodic boundary conditions), we can use the limiting formula for the inverse Kasteleyn matrix, expressed as contour integrals, to obtain an exact (though potentially complicated) analytic expression for the vison correlator. We will apply this approach to analytically determine the asymptotic behavior of the vison correlator along a simple path in the square-octagon lattice in Sec. IV D. For other cases, we can use sparse LU decomposition to efficiently determine the required submatrix of K^{-1} numerically. However, for certain graphs, the Kasteleyn matrix K can be ill-conditioned, meaning it has a large condition number $\kappa = \|K\| \|K^{-1}\|$. We find this to be the case for the Aztec diamond and the square-octagon fortress, as detailed in Appendix C. In such cases, standard floating-point LU factorization is unreliable for numerically computing the required submatrix and can produce highly inaccurate results. To avoid this issue, we implement sparse fraction-free LU factorization [56–58], which relies entirely on exact integer arithmetic. We will refer to fraction-free sparse LU as FFLU for short.

In summary, the numerical procedure for calculating vison correlators along a string E is as follows:

- (i) Construct the Kasteleyn matrix K with integer values and calculate its fraction-free sparse LU decomposition [56].
- (ii) Use the LU factors to perform fraction-free forward and back substitution [57] to calculate the submatrix $(K^{-1})_E$, by solving $Kx = \delta_v$ for each vertex $v \in E$ contained in E , while maintaining the exact rational form of the values.
- (iii) Calculate the determinant in Eq. (10) using floating-point numbers with sufficient precision to account for the condition number κ of the matrix $I_\ell - 2(K')_E(K^{-1})_E$.

If the graph is not bipartite, only minor adjustments are needed: in the second step above, one solves $Kx = \delta_v$ for every vertex in E , and the matrices in Eq. (10)— $I_{2\ell}$, $(K')_E$, and $(K^{-1})_E$ —are of size $2\ell \times 2\ell$, with the final result having the square root of the determinant due to using Pfaffians.

We note that the fraction-free sparse LU method described above is sufficiently efficient that all numerical results presented in this paper, including correlators as small as $< 10^{-20}$, were calculated using plain PYTHON, with each plot generated in under a few hours on a desktop computer. In contrast, calculating the correlators up to a precision of 10^{-5} for the square-octagon lattice dimer model using Monte Carlo calculations shown in Sec. IV required approximately one day on 100 computing cores. Moreover, Monte Carlo convergence for the square-octagon fortress is observed to be slow [59,60]. As a result, calculating correlators on the fortresses via Monte Carlo is extremely computationally expensive, and we therefore do not calculate them using Monte Carlo. This comparison highlights the remarkable efficiency and power of the Kasteleyn matrix-based method for calculating vison correlators. We briefly comment on the path independence of the vison correlator in the absence of monomers. Any contractible vison loop can be decomposed into a product of elementary vison loops around each interior lattice site. Each such factor equals -1 , because each site is touched by exactly one dimer. Therefore, the vison correlators defined along two paths p and p' which are deformable into each other and have the same end points can differ only by an overall minus sign. Since the vison correlator is path independent only up to a sign, we will always consider its absolute value.

III. PHASE SEPARATION EXAMPLE I: AZTEC DIAMOND

A. Square lattice with rectangular boundaries

In this section, we present the spin Hamiltonian that, in the low-energy limit, maps onto a quantum dimer model on a square lattice with rectangular boundaries. This construction is inspired by the Hamiltonians in Refs. [27,46,47]. We also review some of the known results about dimer models on the square lattice with rectangular boundaries.

Consider an $n \times m$ rectangular section of the square lattice, with vertices labeled by pairs (i, j) where $1 \leq i \leq n$ and $1 \leq j \leq m$, as shown in Fig. 6. Place spin-1/2 degrees of freedom on the links of the lattice—these are indicated by the blue dots in the figure. Next, construct the line graph of the square lattice: in this graph, each vertex corresponds to a spin, and two vertices are connected if the associated edges of the original square lattice share a common vertex. This line graph can be interpreted as a graph of corner-sharing polygons, where the polygons in the bulk are

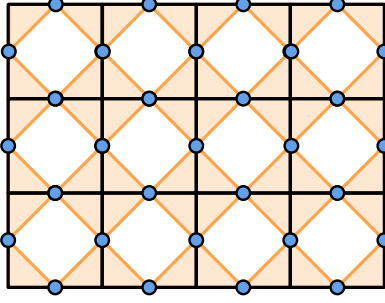


FIG. 6. Square lattice with rectangular boundaries, where edges are shown in black. Blue dots represent spin-1/2 sites. Spins belonging to the same plaquette are connected by orange edges, forming a lattice of corner-sharing polygons, which are shaded in orange.

squares while those on the boundaries are triangles, as illustrated by the orange polygons in Fig. 6. This corner-sharing graph provides a natural graph to define our Hamiltonian, which has two pieces:

$$H_{\text{sq}} = H_{\text{sq},0} + H_{\text{sq},1}, \quad (11)$$

where $H_{\text{sq},0}$ is designed to impose the dimer constraint energetically and $H_{\text{sq},1}$ is designed to generate the ring-exchange and the Rokhsar-Kivelson potential [1]. The classical part of the Hamiltonian, $H_{\text{sq},0}$ is given by

$$H_{\text{sq},0} = U \sum_{p \in \{\diamond, \blacktriangle, \blacktriangledown\}} (S_p^z - h_p)^2, \quad (12)$$

where $S_{\diamond}^z$ denotes the sum of the $S^z \in \{+1/2, -1/2\}$ over the four spins located on the vertices of an orange-shaded square $\diamond$. Similarly, $S_{\blacktriangle}^z$, and $S_{\blacktriangledown}^z$ represent the sum of S^z over the two and three spins on the boundaries of triangles similar to $\blacktriangle$ and $\blacktriangledown$, respectively. We define $h_p \equiv q_p/2 - 1$, where q_p is the number of spins on the boundary of p . Thus, we have $h_{\diamond} = 1$, $h_{\blacktriangle} = 1/2$, and $h_{\blacktriangledown} = 0$. Note that in the sum in Eq. (12), we also include orientations of $\blacktriangle$ and $\blacktriangledown$, obtained by a rotation by 90° , 180° , and 270° , which are present in Fig. 6.

The ground state manifold of $H_{\text{sq},0}$ maps to dimer coverings of the square lattice. Since all terms of $H_{\text{sq},0}$ commute with each other, the ground state manifold can be obtained by minimizing each term in the sum individually. We will see below that this simultaneous minimization can be done, implying that $H_{\text{sq},0}$ is also frustration free. Minimizing the term corresponding to orange squares $\diamond$ gives the constraint $S_{\diamond}^z = 1$ for each $\diamond$, implying that three of the spins have $S^z = +1/2$ and one spin has $S^z = -1/2$ on every $\diamond$. Mapping $S_{\mu}^z = \pm 1/2$ to the absence or presence of a dimer on link μ , we see that $(S_{\diamond}^z - 1)^2$ is minimized when exactly one dimer touches the site at the

center of $\diamond$ giving us the hard-core dimer constraint. It is easy to check that minimizing $(S_p^z)^2$ for $p \in \{\blacktriangle, \blacktriangledown\}$ imposes the hard-core dimer constraint on the boundary sites of the square lattice.

We now describe $H_{\text{sq},1}$, which is designed to map to the ring-exchange and the Rokhsar-Kivelson potential terms [1] when interpreted in terms of dimers. $H_{\text{sq},1}$ is defined as

$$H_{\text{sq},1} = \sum_{\square} \left(V - J \prod_{\nu=1}^4 2S_{\nu}^x \right) \left[\sum_{\eta \in \{\pm\}} \prod_{\mu=1}^4 \left(S_{\mu}^z + \eta \frac{(-1)^{\mu}}{2} \right) \right], \quad (13)$$

where the outer sum runs over all plaquettes $\square$ of the square lattice, and S_1, S_2, S_3, S_4 denote the four spins located on the edges of a square plaquette, taken in a clockwise order. The term in square brackets acts (up to a constant multiple) as a projection operator that selects a flippable plaquette. A plaquette is said to be flippable if it has dimers on a pair of opposite edges. In terms of spin configurations, a plaquette is flippable if $(S_1^z, S_2^z, S_3^z, S_4^z)$ is $(1, -1, 1, -1)/2$ or $(-1, 1, -1, 1)/2$. The term proportional to J flips all four spins on a plaquette, provided the plaquette is flippable, thereby generating the ring-exchange process. The terms proportional to V correspond to the RK potential [1].

In the limit $U \gg |V|, |J|$, the low-energy states are those that correspond to valid dimer coverings of the square lattice. Within this subspace, $H_{\text{sq},1}$ acts as the RK quantum dimer model [1]:

$$H_{\text{sq},1}^{\text{dimer}} = \sum_{\square} -J \left[|\text{II}\rangle \langle \text{II}| + |\text{II}\rangle \langle \text{II}| \right] + V \left[|\text{II}\rangle \langle \text{II}| + |\text{II}\rangle \langle \text{II}| \right], \quad (14)$$

where $|\text{II}\rangle$ and $|\text{II}\rangle$ denote the two flippable dimer configurations on a square plaquette. For $J = V$, this dimer Hamiltonian can be rewritten as a sum of (noncommuting) projectors:

$$H_{\text{sq},1}^{\text{dimer}} = J \sum_{\square} \left[|\text{II}\rangle \langle \text{II}| - |\text{II}\rangle \langle \text{II}| \right] \left[\langle \text{II}| - \langle \text{II}| \right]. \quad (15)$$

For $J > 0$, the ground state of this Hamiltonian is the uniform superposition of all dimer configurations—known as the RK wave function—since it is annihilated by every projector in Eq. (15).

$$|\Psi_{\text{RK}}^{\text{sq}}\rangle = \sum_{\mathcal{C}} |\mathcal{C}\rangle, \quad (16)$$

where the sum runs over all dimer coverings $\mathcal{C}$ of the square lattice.

Certain well-known properties of the RK wave function $|\Psi_{\text{RK}}\rangle$ follow from known results about the classical dimer model on the square lattice with rectangular boundaries. These properties can be derived using Kasteleyn matrix methods [21–23,49], which we reviewed in Sec. II. In particular, the long-distance behavior of the dimer-dimer connected correlator can be computed analytically using Eq. (6). It is known that $C_{\mu\nu}^d$ decays as a power law at long distances: in general, $C_{\mu\nu}^d \propto 1/R_{\mu\nu}^2$, where $R_{\mu\nu}$ denotes the distance between the edges μ and ν [23,61]. (Depending on the relative orientation of the dimers and the vector joining μ and ν , the decay of the dimer-dimer connected correlator may follow a higher power [61].) Since $d_\mu = S_\mu^z + 1/2$, the dimer-dimer connected correlator is equal to the spin-spin connected correlator in the S^z basis.

The power-law decay of the dimer-dimer correlator implies that the quantum dimer model, and hence the spin Hamiltonian in Eq. (11), is at a critical point in the phase diagram. Indeed, the RK point $J = V$ lies at a quantum critical point separating different ordered phases [26,62,63].

To summarize, in the limit $U \rightarrow \infty$, the spin Hamiltonian in Eq. (11) maps onto a quantum dimer model on the square lattice with rectangular boundaries. At the RK point, the system resides at a critical point characterized power-law dimer-dimer connected correlations, separating distinct ordered phases.

B. Aztec diamond

In this section, we consider the spin and dimer models defined on the Aztec diamond. Although this Hamiltonian differs from that on the square lattice with rectangular boundaries in Eq. (11) only by boundary terms, the ground state at the RK point exhibits drastically different properties. This provides our first example of the breakdown of the thermodynamic limit.

The Aztec diamond is a finite region of the square lattice, with boundaries oriented at $\pm 45^\circ$ relative to the lattice basis vectors, such that each corner is one square wide, as shown in Fig. 7. As with the square lattice with rectangular boundaries, we place the spin-1/2 s on the edges of the Aztec diamond and construct the line graph of the Aztec diamond. This gives us a graph composed of corner-sharing polygons, as shown in Fig. 7. The spin Hamiltonian on the Aztec diamond is closely related to that in Eq. (11) and is defined as

$$H_{\text{az}} = H_{\text{az},0} + H_{\text{az},1}, \quad (17)$$

where

$$H_{\text{az},0} = U \sum_{p \in \{\diamond, \blacktriangle\}} (S_p^z - h_p)^2. \quad (18)$$

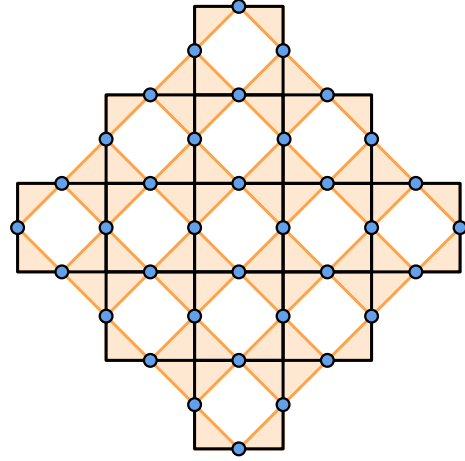


FIG. 7. The black edges define an Aztec diamond. Spin-1/2 degrees of freedom (blue dots) are located at the midpoints of these edges, forming a square lattice with square boundaries. As in Fig. 6, we construct the line graph of the Aztec diamond, resulting in a graph of corner-sharing polygons, shaded in orange. In this construction, the spins are naturally viewed as residing on the vertices of the resulting graph.

Here, the sum runs over all plaquettes of the shape $\diamond$ and the various orientations of $\blacktriangle$. Symbolically, $H_{\text{az},1}$ is given by the same expression as $H_{\text{sq},1}$ in Eq. (13), except that the sum is now taken over the plaquettes of the Aztec diamond rather than the rectangle. In the limit $U \gg |V|, |J|$, the ground-state manifold of $H_{\text{az},0}$ consists of dimer coverings of the Aztec diamond, and in terms of dimers, $H_{\text{az},1}$ corresponds to the RK Hamiltonian. As before, for $V = J$, the RK Hamiltonian becomes a sum of projectors, and a ground state is the RK wave function $|\Psi_{\text{RK}}^{\text{az}}\rangle$ on the Aztec diamond. Notably, $H_{\text{az},0}$ differs from $H_{\text{sq},0}$ only at terms which are at the boundaries of the two graphs.

To understand the properties of the RK wave function on the Aztec diamond, we first calculate the dimer density $\langle d_\mu \rangle$ using the Kasteleyn method described in Sec. II A, specifically applying Eq. (4) with $k = 1$. In agreement with the infinite-limit asymptotics proved in Ref. [6], the behavior stands in a stark contrast to that of the square lattice with rectangular boundaries, where the dimer density remains constant in the bulk, $\langle d_\mu \rangle = 1/4$ for all edges. As briefly discussed in Sec. I, the Aztec diamond features “frozen” corners: certain links are occupied, while others are not occupied, with a probability approaching one in the infinite system-size limit [3,6]. In a typical configuration, these frozen corners exhibit a staggered dimer pattern, as illustrated in Fig. 1 and its inset. Inside the circular region shown in the same figure, however, the dimers are not frozen. This central area, labeled as the critical region is separated from the frozen corners by a boundary known in the mathematical literature as the Arctic circle [3,6], since it separates the frozen and the “liquid” regions. It is also known that, inside the Arctic circle, the

dimer-dimer connected correlator decays as $1/(\text{distance})^2$ [5,6,34,36,42] similar to the behavior in the square lattice with rectangular boundaries.

The above results imply that, in the spin system, the corner regions are in an ordered phase, while the region inside the Arctic circle is in a critical phase. Importantly, the frozen regions occupy a finite fraction of the Aztec diamond (specifically $1 - \pi/4 \approx 21\%$) indicating that this is not merely a boundary effect. To the best of our knowledge, this quantum phenomenon—where a change in the shape of the boundaries gives rise to distinct spatial regions residing in different quantum phases—has not been reported in the literature. We refer to this effect as *quantum phase separation*. This phenomenon bears resemblance to classical phase coexistence, such as the simultaneous presence of liquid and solid phases in systems undergoing a first-order transition, although in our case the phase separation is induced purely by the geometry of the boundaries. Additionally, we note that the dimers in the top and the bottom corners are ordered horizontally, while those in the left and right corners are oriented vertically.

So far we have explained the coexistence of frozen and critical (or liquid) regions in the ground state at the special RK point $V = J$ of our Hamiltonian Eq. (17). A natural question arises: what happens when we move away from this point? Since the region inside the Arctic circle is critical, it remains unclear whether quantum phase separation is unique to the RK point or persists over an extended region of the phase diagram. It is conceivable that even an infinitesimal deviation from the RK point causes the critical region to transition into an ordered phase, similar to the square lattice with rectangular boundaries. If this order is the same as the staggered order of the frozen corners, then it is possible that the perturbed system will have a single ordering with no phase separation. If this is the case, quantum phase separation would occur only at a single fine-tuned point in the phase diagram. However, if the order assumed by the critical region upon perturbation from the RK point is different from the frozen corners, then there will be two macroscopic regions with distinct phases. We expect there to be a critical region between these two ordered regions. Quantum Monte Carlo simulations are required to be done away from the RK point to say conclusively about the fate of phase separation, which we plan to perform in a subsequent publication. Because of the critical nature of the region inside the arctic circle, it is not clear if the phase separation survives perturbations away from the RK point. However, if the system exhibited phase separation between two (or more) regions with exponentially decaying correlations (i.e., gapped phases), one would expect stability under small perturbations away from the RK point, since the gap cannot close abruptly. In Sec. V, we present an example of such a system on the square-octagon fortress, featuring three distinct regions: two with exponentially decaying (connected) dimer

correlations and one with critical correlations. Before turning to that, however, we first study a model on a simpler graph: the square-octagon lattice with rectangular boundaries.

IV. SQUARE-OCTAGON LATTICE WITH RECTANGULAR BOUNDARIES

A. Hamiltonian

We now describe the square-octagon lattice (also known as the “truncated square tiling”) and introduce the spin Hamiltonian that maps onto a quantum dimer model defined on this lattice.

The square-octagon lattice, composed of alternating squares surrounded by octagons, is shown in Fig. 8. In this section, we focus on square-shaped regions of this lattice like the one displayed in Fig. 8 and we simply refer to such sections as the square-octagon lattice. Analogous to Sec. III, we construct its line graph to obtain a graph of corner-sharing triangles, on which we define a spin Hamiltonian. In this line graph, each vertex represents an edge of original lattice, and two vertices are connected if and only if their corresponding edges in the original lattice share a common end point. The Hamiltonian, analogous to Eqs. (11)–(13), for the square-octagon lattice is given by

$$H_{\text{sos}} = H_{\text{sos},0} + H_{\text{sos},1}, \quad (19)$$

where $H_{\text{sos},0}$ energetically enforces the dimer constraint, while $H_{\text{sos},1}$ generates the RK Hamiltonian. Note that “sos”

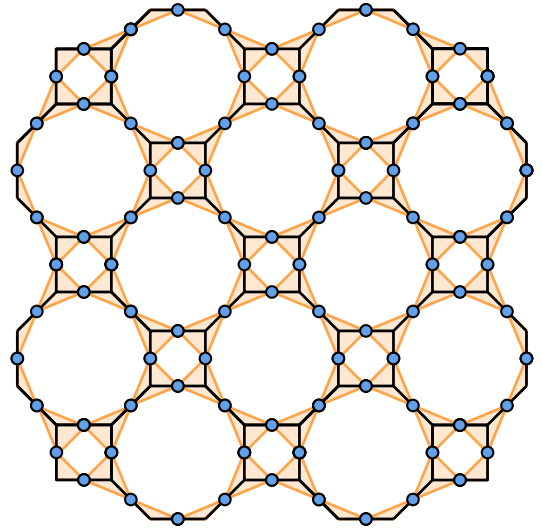


FIG. 8. The black lines form a square-octagon lattice with a square boundary. Blue dots represent the spin-1/2 degrees of freedom, located at the vertices of the line graph of the square-octagon lattice. The edges of this line graph are marked in orange. This line graph can be viewed as a graph of corner-sharing triangles, which are shaded in orange.

here refers to “square-octagon with square boundaries.” We define $H_{\text{sos},0}$ as

$$H_{\text{sos},0} = U \sum_{p \in \{\triangle, \blacktriangle, \blacktriangledown\}} (S_p^z - h_p)^2, \quad (20)$$

where S_p^z is the sum of the S^z over all spins on triangle p , and $h_p \equiv 1 - q_p/2$, as in Sec. III. Explicitly, $h_{\triangle} = -1/2$, while $h_{\blacktriangle} = h_{\blacktriangledown} = 0$. We define $H_{\text{sos},1}$ as

$$H_{\text{sos},1} = \sum_{\square} \left(V_4 - J_4 \prod_{\nu=1}^4 2S_{\nu}^x \right) \left[\sum_{\eta \in \pm\mu=1}^4 \left(S_{\mu}^z + \eta \frac{(-1)^{\mu}}{2} \right) \right] \\ + \sum_{\bigcirc} \left(V_8 - J_8 \prod_{\nu=1}^8 2S_{\nu}^x \right) \left[\sum_{\eta \in \pm\mu=1}^8 \left(S_{\mu}^z + \eta \frac{(-1)^{\mu}}{2} \right) \right], \quad (21)$$

with the first sum running over all square plaquettes and the second over all octagonal plaquettes. Here, S_1^z, S_2^z, S_3^z , and S_4^z in the first sum refer to the spins along a square plaquette (ordered clockwise), and $S_1^z, S_2^z, \dots, S_8^z$ in the second sum refer to the spins along an octagonal plaquette (also ordered clockwise).

In the limit $U \gg |V_4|, |V_8|, |J_4|, |J_8|$, $H_{\text{sor},0}$ imposes the dimer constraint is energetically, and the low-energy manifold consists of perfect dimer coverings of the lattice. Within this manifold, $H_{\text{sor},1}$ acts as the RK Hamiltonian:

$$H_{\text{sos},1}^{\text{dimer}} = \sum_{\square} -J_4 \left[|\text{dimer}\rangle \langle \text{dimer}| + |\text{dimer}\rangle \langle \text{dimer}| \right] \\ + V_4 \left[|\text{dimer}\rangle \langle \text{dimer}| + |\text{dimer}\rangle \langle \text{dimer}| \right] \\ + \sum_{\bigcirc} -J_8 \left[|\text{dimer}\rangle \langle \text{dimer}| + |\text{dimer}\rangle \langle \text{dimer}| \right] \\ + V_8 \left[|\text{dimer}\rangle \langle \text{dimer}| + |\text{dimer}\rangle \langle \text{dimer}| \right]. \quad (22)$$

For $V_4 = J_4 > 0$, $V_8 = J_8 > 0$, and arbitrary V_4/V_8 , $H_{\text{sos},1}^{\text{dimer}}$ becomes a sum of (noncommuting) projectors, and the uniform superposition of all dimer coverings, $|\Psi_{\text{RK}}^{\text{sos}}\rangle$, is the ground state. It is known that the ring-exchange moves on the square-octagon lattice are ergodic [59,60], implying that all dimer coverings belong to a single connected sector. As a result, the ground state of Eq. (22) at the RK point is unique.

To understand the properties of the RK wave function on the square-octagon lattice, we will compute the dimer-dimer and vison correlators using Kasteleyn-like methods.

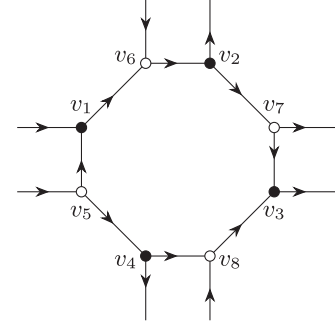


FIG. 9. Square-octagon fundamental domain with eight vertices $v_1, \dots, v_8$. The Kasteleyn orientation, indicated by arrows on the edges, is inherited from the square lattice: by “flattening” the octagon—lowering vertices v_6 and v_2 to align with v_1 , and raising v_4 and v_8 to align with v_5 —the square-octagon lattice is realized as a subgraph of the square lattice (see also Fig. 22).

B. Inverse Kasteleyn matrix asymptotics

In this section, we compute the asymptotic forms of the partition function and the inverse Kasteleyn matrix in the infinite-size limit for the square-octagon lattice with rectangular boundaries and periodic boundary conditions (PBC). These asymptotics are later used in Secs. IV C and IV D to evaluate the dimer-dimer and vison correlators, respectively. This follows standard methods, as described for example in Refs. [42,64]. Here, we describe only the key definitions, the fundamental domain (unit-cell) diagram, and final results, deferring the full derivation to Appendix B.

Figure 9 shows a fundamental domain of the square-octagon lattice, with eight vertices labeled $v_1, \dots, v_8$, and a Kasteleyn orientation indicated by the arrows on each edge. We construct the graph G_n by taking n horizontal and n vertical translates of the fundamental domain. For analytical convenience, we impose periodic boundary conditions, though the resulting infinite-limit asymptotics agree with the finite-size, open-boundary numerical calculations. We label vertex coordinates in G_n as triples $[x, y, s]$, where $(x, y) \in \{0, \dots, n-1\}^2$ identifies the translated copy of the fundamental cell, and $s \in \{1, \dots, 8\}$ specifies the vertex $v_1, \dots, v_8$ within the cell.

Correlators of diagonal operators in the RK wave function $|\Psi_{\text{RK}}^{\text{sos}}\rangle$ are equal to the correlators of a classical dimer model on the square-octagon lattice. Since all dimer coverings occur in $|\Psi_{\text{RK}}^{\text{sos}}\rangle$ with equal probabilities, the partition function of the classical dimer model Z_n , is simply

$$Z_n = \#\{\text{dimer configurations of } G_n\}. \quad (23)$$

Because the graph G_n is embedded on a torus, counting the number of dimer coverings requires determining four specific Kasteleyn matrices: $K_n^{00}, K_n^{01}, K_n^{10}$, and K_n^{11} [21]. The partition function can then be expressed as

$$Z_n = \frac{1}{2}(-Z_n^{00} + Z_n^{01} + Z_n^{10} + Z_n^{11}), \quad (24)$$

where $Z_n^{\alpha\beta} = \det K_n^{\alpha\beta}$. As described for general graphs in [42], §3], the Kasteleyn matrices $K_n^{\alpha\beta}$ can be block-diagonalized via a Fourier transform. This allows using a Riemann sum approximation to evaluate quantities such as the limiting free energy per unit cell, $\lim_{n \rightarrow \infty} n^{-2} \log Z_n$

as a double contour integral. The limiting entries of $(K_n^{\alpha\beta})^{-1}$, for $\alpha\beta = 00, 01, 10, 11$, which are needed to analytically calculate the dimer and vison correlators, are also determined similarly. From the block diagonalization of $K_n^{\alpha\beta}$, we obtain (see Appendix B) that, in the limit $n \rightarrow \infty$, the matrix entries $\langle 0, 0, s | K_n^{\alpha\beta} | x, y, t \rangle$ for any of the $\alpha\beta$ converge to

$$\langle 0, 0, s | \mathcal{K}^{-1} | x, y, t \rangle := \begin{cases} \int_0^{2\pi} \int_0^{2\pi} \frac{Q_{st}(e^{ik_x}, e^{ik_y}) e^{-i(k_x x + k_y y)}}{-5 + 2 \cos k_x + 2 \cos k_y} \frac{dk_x}{2\pi} \frac{dk_y}{2\pi}, & s, t \text{ different color vertices} \\ 0, & s, t \text{ same color vertices} \end{cases}, \quad (25)$$

where $Q_{st}(z, w) = -Q_{ts}(z, w)$ is a rational function given by the entries in (26)

$s \backslash t$	1	2	3	4
5	$2 - w^{-1}$	$1 - z^{-1}w^{-1}$	$1 - 2z^{-1}$	$-z^{-1} - w + 1$
6	$z + w - 1$	$2 - z^{-1}$	$1 - wz^{-1}$	$1 - 2w$
7	$2z - 1$	$z + w^{-1} - 1$	$2 - w$	$1 - zw$
8	$1 - zw^{-1}$	$1 - 2w^{-1}$	$-z^{-1} - w^{-1} + 1$	$z - 2$

(26)

whose rows are indexed by $s = 5, 6, 7, 8$ and columns by $t = 1, 2, 3, 4$. (As seen in Fig. 9, the vertices v_s and v_t can be split into different colors with $s \in \{5, 6, 7, 8\}$ and $t \in \{1, 2, 3, 4\}$.) By translational invariance, this also determined the matrix entries for any pair of vertices $|w, z, s\rangle$ and $|x, y, t\rangle$. Equation (25) exemplifies the more general fact that the matrix entries of the limiting $\mathcal{K}^{-1}$ are always given by contour integrals which give Fourier coefficients of one of finitely many trigonometric polynomials [42] (Sec. IV). The integrals in Eq. (25) can be reduced to a single integral using the residue theorem, as detailed in Appendix B.

It is well known that the total number of dimer coverings can be expressed as the partition function of a free-fermion hopping model defined on the same lattice as the dimer model [31], providing a physics-friendly interpretation of Eq. (25). With periodic boundary conditions, the system exhibits translational invariance, allowing diagonalization of the free-fermion model in momentum space. For each momentum mode, one obtains an 8×8 “Hamiltonian,” whose eigenvalues will give eight band dispersions. The Green’s function in the momentum space is obtained by inverting this momentum dependent Hamiltonian. Doing so will lead to the appearance of the determinant of the Hamiltonian in the denominator, which is a product of the eight band dispersions given by the denominator of the integrand in Eq. (25): $-5 + 2 \cos k_x + 2 \cos k_y$. The real-space Green’s function, $\langle 0, 0, s | \mathcal{K}^{-1} | x, y, t \rangle$, is obtained by performing a Fourier transform of the momentum space

Green’s function. The factor $Q_{st}(e^{ik_x}, e^{ik_y})$ in Eq. (25) arises from the sublattice structure.

Having determined the inverse Kasteleyn matrix elements in the infinite-system limit, we now use them to calculate the dimer-dimer and the vison correlators in the following sections.

C. Dimer-dimer connected correlator

In this section, we calculate the dimer-dimer connected correlator $C_{\mu\nu}^d$ along the four paths shown in Fig. 10. A general argument from Ref. [42] shows that exponential vs power-law decay of the dimer-dimer connected correlator is determined by the *characteristic polynomial* $P(z, w)$ of the lattice, which for the square-octagon lattice is given by $P(z, w) = -5 + z + z^{-1} + w + w^{-1}$. We explain this interpretation below. The dimer-dimer connected correlator is given in terms of the inverse Kasteleyn matrix according to Eq. (6). In the infinite-size limit, we replace the matrix elements of the finite inverse Kasteleyn matrix in Eq. (6) with those of the infinite inverse Kasteleyn matrix $\mathcal{K}^{-1}$ defined in Eq. (25) (see Appendix A for details). The denominator of the integrand in Eq. (25) is the characteristic polynomial $P(z, w)$, with $z = e^{ik_x}$ and $w = e^{ik_y}$. Since for $k_x, k_y \in [0, 2\pi)$, the square-octagon lattice $P(e^{ik_x}, e^{ik_y})$ does not have any zeros, and $Q_{st}(e^{ik_x}, e^{ik_y})$ is analytic, the integrand of Eq. (25) is an analytic function of k_x and k_y . Thus its Fourier transform written in Eq. (25) will decay exponentially in $|x|$ and $|y|$.

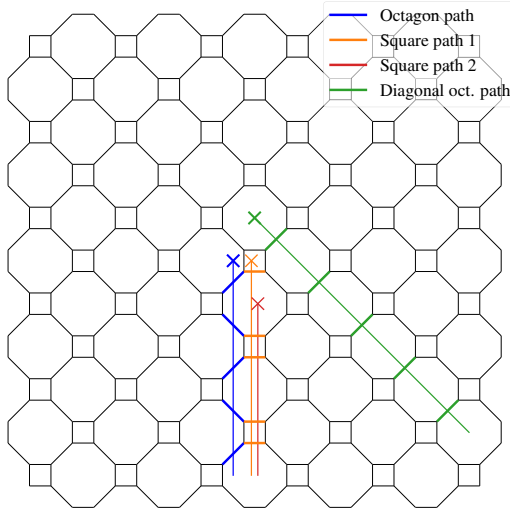


FIG. 10. Diagram of the four paths considered on the square-octagon lattice, drawn on a lattice with radius $R = 6$. Here, “radius” refers to the number of edges crossed by a line starting from the center square and going up vertically. The two square paths, shown in similar colors (orange and red), differ only in their starting point: one begins on a square face, and the other on an octagon face. We refer to the longer of the two as “square path 1.” The “octagon path” and “diagonal octagon path” go through octagon faces only, with the former referring to horizontal or vertical paths and the latter to a diagonal path. These paths cross only diagonal edges which border the octagon faces.

This argument translated in the language of the free fermion model goes as follows: the product of band dispersion of the free fermions is given by $P(e^{ik_x}, e^{ik_y}) = -5 + 2 \cos k_x + 2 \cos k_y$. Since this function has a gap (it never vanishes for real k_x, k_y), all the bands of the free fermion model are gapped and the real-space Green’s function and thus the dimer-dimer connected correlator will decay exponentially with distance.

We can also obtain the exact decay rates and correlation lengths using the following standard result:

Lemma IV.1. If f is 2π periodic and real analytic with analytic extension to a neighborhood of the strip $\{z \in \mathbb{C} : |\text{Im } z| \leq \kappa\}$ for some $\kappa > 0$, then the Fourier coefficients $\hat{f}(\xi) = (1/[2\pi]) \int_0^{2\pi} f(x) e^{-i\xi x} dx$ satisfy

$$|\hat{f}(\xi)| \leq C e^{-\kappa|\xi|}, \quad (27)$$

for some constant $C = C(f)$. Conversely, if the Fourier coefficients have the above exponential decay, then f has analytic extension to the strip $\{z \in \mathbb{C} : |\text{Im } z| < \kappa\}$.

Since the double integrals in Eq. (25) can be reduced to single integrals [see, e.g., Eq. (B20)], the one-dimensional case stated above is enough. More generally, a d -dimensional version can be formulated, see, for example, Ref. [65] (Lemma 5.6).

Applying the single integral expression Eq. (B20) to Eq. (25), we see that the resulting integrand will always have denominator $\sqrt{(5 - 2 \cos \theta)^2 - 4}$. When extended to the complex plane, the nearest zero of this denominator to the real line occurs when $\cos(z) = 3/2$, i.e., at $z = \arccos(3/2) = -\log[(3 - \sqrt{5})/2]i$. Now, applying the lemma, we find that

$$|\langle 0, 0, s | \mathcal{K}^{-1} | x, y, t \rangle| \leq C \left(\frac{3 - \sqrt{5}}{2} \right)^{\max(|x|, |y|)(1-\varepsilon)}, \quad (28)$$

for any $\varepsilon > 0$ and a (possibly different) constant C .

For numerical comparison, it is convenient to index distances using the “edge distance” ℓ , measured by counting the number of edges traversed, rather than by fundamental cell translations. Since the four paths we consider pass through two edges per fundamental cell, this introduces a factor of $1/2$ in the exponent. By the formula for the dimer-dimer connected correlator Eq. (6), the bound Eq. (28) implies an upper bound on the dimer-dimer correlation length ξ with respect to the edge distance ℓ :

$$\xi \leq -\log \left(\frac{3 - \sqrt{5}}{2} \right)^{-1} = 1.039043\dots \quad (29)$$

In fact, along a horizontal or vertical line, indexing the dimers in the path by $\ell \in \mathbb{N}$ and applying Eq. (6) and the converse statement Lemma IV.1 gives the asymptotic correlation length to actually be $\xi = -\log[(3 - \sqrt{5})/2]^{-1}$.

We compare the analytically obtained exponential decay in Eq. (29) to the numerical results for finite-size systems shown in Fig. 11. For direct comparison with the best-fit slopes, we note that the reciprocal $-\log[(3 - \sqrt{5})/2] = 0.962424\dots$ provides a lower bound on the inverse correlation length. The numerical best-fit slopes for the octagon and square paths are all in the range 0.978–0.991, which show close agreement with the above value, as expected since the bound is attained along these paths in the infinite size limit.

Let us briefly contrast the above with the *square* lattice, where the corresponding denominator is the characteristic polynomial $P(z, w) = 4 + z + z^{-1} + w + w^{-1}$, which *does* have a zero on the unit circles at $z = w = -1$. As shown in Ref. [64] (and more generally in Sec. 4.2.2 of Ref. [42]), this implies that the analogue of the integral in Eq. (25) decays according to a power law, leading to power-law decay of the dimer correlator. In terms of the associated free-fermion model on the square lattice, the band dispersion $4 + 2 \cos k_x + 2 \cos k_y$ is gapless at $(k_x, k_y) = (\pi, \pi)$ in the Brillouin zone, which explains power-law decay of the dimer-dimer correlator. A similar phenomenon occurs on the hexagonal lattice, which is also critical. More generally, since the characteristic polynomial $P(z, w)$ can

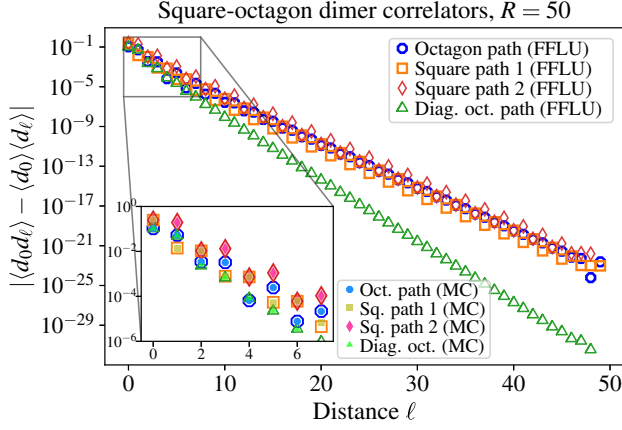


FIG. 11. Log plot of the dimer-dimer connected correlator along the four paths depicted in Fig. 10, calculated using the fraction-free LU (FFLU) method and compared against Monte Carlo (MC) data (inset). The lattice has radius $R = 50$, meaning there are 50 edges along a horizontal or vertical path from the center to the boundary, corresponding to a graph with 19 996 vertices. All dimer correlators show exponential decay. The best-fit inverse correlation lengths (given by the negative slopes of the log plot) lie in the range 0.978–0.991 for the first three paths (calculated over the range $\ell = 30$ to 46), and 1.405 for the fourth path in the same ℓ range. These inverse correlation lengths are calculated with respect to the edge distance ℓ , and are to be compared with the infinite limit lower bound $-\log([3 - \sqrt{5}]/2) = 0.962424$.

be quickly computed from the fundamental cell, one can readily check whether a periodic lattice exhibits exponential or power-law decay of correlations [42]. For example, the characteristic polynomials for a number of different lattices were calculated in Ref. [66].

D. Vison correlator

From the exponential decay of the dimer-dimer correlator, we infer that the quantum dimer model shown in Eq. (22) is likely not at a critical point, unlike the square lattice RK dimer model. To determine the phase of the dimer model, we review the connection between gauge theories and dimer models.

It is well known that quantum dimer models can be effectively described by gauge theories [27,43]. Gauge theories can either be in a deconfined phase, corresponding to the dimer model being in a quantum spin liquid phase, or in a confined phase, corresponding to an ordered phase such as a valence bond solid (VBS). In particular, the dimer models studied in this paper can be mapped to $\mathbb{Z}_2$ gauge theories, which feature both electric and flux (vison) excitations. The dimer constraint at each site plays the role of a Gauss law in the gauge theory, while electric charges correspond to violations of this constraint (i.e., sites with the incorrect number of dimers). Visions are flux excitations that always appear in pairs, and the vison operator associated with a given path creates a pair of

visions at its end points. If the $\mathbb{Z}_2$ gauge theory is in the deconfined (gapped) phase, both the dimer-dimer and vison correlators decay exponentially with distance, and the visions behave as well-defined particlelike excitations. Moreover, the exponential decay of the vison correlator to zero as the string length increases necessarily implies that the charges are fractionalized [29]. However, if the vison correlator approaches a nonzero constant, it indicates that the gauge theory is in the confined phase and the dimer model is in an ordered phase. This behavior can be directly checked, for example, in the square lattice RK dimer model [1]. For RK potentials much larger than the ring-exchange coupling, the system exhibits columnar or staggered order, depending on the sign of the RK potential. When the ring-exchange coupling is exactly zero, it is straightforward to see that the vison correlator is a constant in the staggered and the columnar configurations. Even when the ring-exchange coupling is small (compared to the RK potential), the system remains ordered, and the vison correlator still approaches a nonzero constant.

Using Eq. (10), we numerically calculate the vison correlator along several paths on a square-shaped section of the square-octagon lattice, similar to the one shown in Fig. 10. The figure also shows the four paths along which we calculate the vison correlator. We fix one end point near the center of the graph and vary the other to generate strings of different lengths. The resulting vison correlators are plotted in Fig. 12. We find that the vison correlator behaves differently depending on the path. Specifically, it remains constant along the octagon and diagonal octagon paths, decays exponentially along square path 1, and shows mixed behavior along square path 2: decaying exponentially if the end point lies on a square plaquette, but remaining constant if it ends on an octagonal plaquette. Since the vison correlator depends only on the end points—not the specific path—the constant value along the octagon path implies it is also constant along square path 2 when both end points lie on octagons. Since the vison correlator approaches a constant along certain paths, the system is not in a $\mathbb{Z}_2$ spin liquid phase and is instead in an ordered phase.

We now analytically prove that the vison correlator converges to a constant along the octagon path in the infinite-size square-octagon lattice with periodic boundary conditions. Our final result is that the vison correlator along the octagon path approaches a constant as the path length goes to infinity:

$$\lim_{\ell \rightarrow \infty} |\langle v_0 v_\ell \rangle| = 0.774\,596\,669\dots \quad (30)$$

To show this, we use vertex coordinates (x, y, t) , where $(x, y) \in \mathbb{Z}^2$ denotes the shift of the fundamental cell and $t \in \{1, \dots, 8\}$ labels the vertex within the cell, following the numbering in Fig. 9. The octagon path can be taken as the path crossing the $v_4 v_5$ and $v_1 v_6$ edges of fundamental cells with (x, y) coordinates $(0, y)$ for $y = 0, 1, 2, \dots$. The other

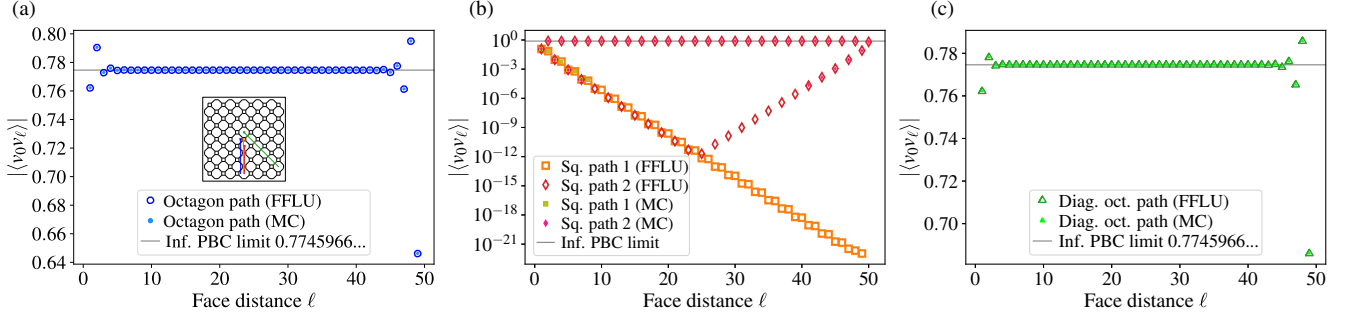


FIG. 12. Vison correlator along different paths [drawn in the inset of (a) and in Fig. 10] in the square-octagon lattice with open rectangular boundary conditions, calculated using fraction-free LU (FFLU) and Monte Carlo (MC) methods. All calculations were carried out on a lattice with a radius $R = 50$. The x-axis in these plots is the number of edges crossed by the paths, denoted ℓ . (a) Vison correlator along the octagon path from Fig. 10, showing close agreement among FFLU, Monte-Carlo, and the analytically calculated infinite-size limit Eq. (30) indicated by the black horizontal line. (b) Vison correlators along the two square paths, which show a mixture of constant and exponential decay behavior. For this plot, square path 2 is taken from the same starting face as in Fig. 10, but continues to the top edge instead of the bottom, making it slightly longer. The Monte Carlo data are plotted for values exceeding 2×10^{-5} , where it agrees well with the FFLU results. For the “square path 1,” represented by orange square markers, the vison correlator decays exponentially with string length l . Fitting a straight line to the log plot over the range $\ell = 20$ to 40, we obtain an inverse correlation length of 0.9955 from the negative of the slope. (c) Vison correlator along the “diagonal octagon path,” again showing close agreement among FFLU, Monte Carlo, and the analytic infinite-size limit. We note that for the octagon path shown in blue, similar plots can be efficiently generated for much larger radii (e.g., $R = 100, 200, 500$) using sparse floating-point LU decomposition, all within a few minutes on a standard laptop.

vertical or horizontal octagon paths are equivalent by translational and reflection symmetry. Recall that to analytically calculate the vison correlator using Eq. (10), we require the submatrices $(\mathcal{K}^{-1})_E$ and $(\mathcal{K}')_E$. To determine these, we first calculate the relevant matrix elements of $\mathcal{K}^{-1}$ using the infinite-size limit expression given in Eqs. (25) and (26), along with the single-integral simplification in Eq. (B20). The required matrix elements are

$$\begin{aligned}
 \langle 0, 0, 5 | \mathcal{K}^{-1} | 0, y, 4 \rangle &= -\langle 0, 0, 6 | \mathcal{K}^{-1} | 0, y, 1 \rangle \\
 &= -\int_0^{2\pi} e^{-i\theta y} F_1(\theta) \frac{d\theta}{2\pi}, \\
 \langle 0, 0, 5 | \mathcal{K}^{-1} | 0, y, 1 \rangle &= -\langle 0, 0, 6 | \mathcal{K}^{-1} | 0, y+1, 4 \rangle \\
 &= -\int_0^{2\pi} e^{-i\theta y} F_2(\theta) \frac{d\theta}{2\pi},
 \end{aligned} \tag{31}$$

where $F_1(\theta)$ and $F_2(\theta)$ are defined as

$$\begin{aligned}
 F_1(\theta) &\equiv \frac{-3 - 2e^{i\theta} + 2\cos\theta + \sqrt{(5 - 2\cos\theta)^2 - 4}}{2\sqrt{(5 - 2\cos\theta)^2 - 4}}, \\
 F_2(\theta) &\equiv \frac{2 - e^{-i\theta}}{\sqrt{(5 - 2\cos\theta)^2 - 4}}.
 \end{aligned} \tag{32}$$

Note that by translational invariance, $\langle 0, y_1, t | \mathcal{K}^{-1} | 0, y_2, s \rangle = \langle 0, 0, t | \mathcal{K}^{-1} | 0, y_2 - y_1, s \rangle$. Thus, the four matrix elements above are sufficient to obtain all the required entries along the octagon path. Thus we have,

$$\begin{aligned}
 \langle 0, y_1, 5 | \mathcal{K}^{-1} | 0, y_2, 4 \rangle &= -\langle 0, y_1, 6 | \mathcal{K}^{-1} | 0, y_2, 1 \rangle \\
 &= -\hat{F}_1(y_2 - y_1), \\
 \langle 0, y_1, 5 | \mathcal{K}^{-1} | 0, y_2, 1 \rangle &= -\langle 0, y_1, 6 | \mathcal{K}^{-1} | 0, y_2 + 1, 4 \rangle \\
 &= -\hat{F}_2(y_2 - y_1),
 \end{aligned} \tag{33}$$

where $\hat{F}_{1,2}$ denotes the Fourier transform of $F_{1,2}$. To obtain the vison correlator along the octagon path, we take the string of edges in Eq. (10) to be $(v_4, v_5), (v_1, v_6)$, followed by their vertical translations. The submatrix $(\mathcal{K}^{-1})_E$ is given by

$$(\mathcal{K}^{-1})_E = \begin{matrix} & \begin{matrix} 0, 4 & 0, 1 & 1, 4 & 1, 1 & \cdots & \ell-1, 4 & \ell-1, 1 \end{matrix} \\ \begin{matrix} 0, 5 \\ 0, 6 \\ 1, 5 \\ 1, 6 \\ \vdots \\ \ell-1, 5 \end{matrix} & \left[\begin{array}{cccccc} -\hat{F}_1(0) & -\hat{F}_2(0) & -\hat{F}_1(1) & -\hat{F}_2(1) & \cdots & -\hat{F}_1(\ell-1) & -\hat{F}_2(\ell-1) \\ \hat{F}_2(-1) & \hat{F}_1(0) & \hat{F}_2(0) & \hat{F}_1(1) & \cdots & \hat{F}_2(\ell-2) & \hat{F}_1(\ell-1) \\ -\hat{F}_1(-1) & -\hat{F}_2(-1) & -\hat{F}_1(0) & -\hat{F}_2(0) & \cdots & -\hat{F}_1(\ell-2) & -\hat{F}_2(\ell-2) \\ \hat{F}_2(-2) & \hat{F}_1(-1) & \hat{F}_2(-1) & -\hat{F}_1(0) & \cdots & \hat{F}_2(\ell-3) & \hat{F}_1(\ell-2) \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \hat{F}_2(-\ell) & \hat{F}_1(-\ell+1) & \hat{F}_2(-\ell+1) & \hat{F}_1(-\ell+2) & \cdots & \hat{F}_2(-1) & \hat{F}_1(0) \end{array} \right] \end{matrix}, \quad (34)$$

where the row and column labeling (y, t) is shorthand for vertex coordinates $(0, y, t)$.

The next quantity needed to calculate the vison correlator using Eq. (10) is the submatrix $(\mathcal{K}')_E$. Here, $\mathcal{K}'$ refers to the infinite-size limit of K' as defined in Eq. (9). The submatrix $(\mathcal{K}')_E$ can be directly read from Fig. 9; it is simply a diagonal matrix with alternating entries $-1, 1, -1, 1, \dots$, in the same basis as $(\mathcal{K}^{-1})_E$ shown in Eq. (34). Multiplying $(\mathcal{K}')_E$ against $(\mathcal{K}^{-1})_E$ flips the signs of every other row, giving a Toeplitz matrix $(\mathcal{K}')_E(\mathcal{K}^{-1})_E$. This Toeplitz matrix is generated by a periodic function F , whose Fourier coefficients are given by interweaving those of F_1 and F_2 , i.e.,

$$\begin{aligned} F(\theta) &= \sum_{j \in \mathbb{Z}} \hat{F}_1(j) e^{i2j\theta} + \sum_{j \in \mathbb{Z}} \hat{F}_2(j) e^{i2j\theta} e^{i\theta} \\ &= F_1(2\theta) + e^{i\theta} F_2(2\theta). \end{aligned} \quad (35)$$

Thus, Eq. (10) [or more accurately Eq. (A8) in the infinite-size limit] gives the vison correlator as

$$\langle (-1)^{\eta_E} \rangle = \det(I_\ell - 2T_\ell(F)), \quad (36)$$

where $T_\ell(F)$ is the $\ell \times \ell$ Toeplitz matrix with matrix elements $[T_\ell(F)]_{ij} = \hat{F}(j-i)$, where the Fourier coefficients are given by $\hat{F}(j) = [1/(2\pi)] \int_0^{2\pi} F(\theta) e^{-ij\theta} d\theta$. The limit of the determinant as $\ell \rightarrow \infty$ can be evaluated using the strong Szegő limit theorem for Toeplitz matrices [67–71].

Theorem IV.1. (Strong Szegő limit theorem) Let $f: \mathbb{R}/(2\pi\mathbb{Z}) \rightarrow \mathbb{C}$ be a smooth function which has no zeros and has winding number zero, and let $T_\ell(f)$ be the Toeplitz matrix with elements $[T_\ell(f)]_{ij} = \hat{f}(j-i)$, where $i, j \in \{0, 1, 2, \dots, \ell-1\}$. If $\hat{c}_k = [1/(2\pi)] \int_0^{2\pi} e^{-ik\theta} \log f(\theta) d\theta$ are the Fourier coefficients of $\log F \in L^1$, then

$$\lim_{\ell \rightarrow \infty} \frac{\det T_\ell(f)}{e^{(\ell+1)\hat{c}_0}} = \exp\left(\sum_{k=1}^{\infty} k \hat{c}_{-k} \hat{c}_k\right). \quad (37)$$

In our case, the symbol is

$$f(\theta) = 1 - 2F(\theta) = \frac{3 + 2e^{2i\theta} + 2e^{-i\theta} - 4e^{i\theta} - 2\cos(2\theta)}{\sqrt{(5 - 2\cos(2\theta))^2 - 4}}. \quad (38)$$

Since $\text{Re}[1 - 2F(\theta)] > 0$ for all θ , the symbol is nonzero and has winding number zero, ensuring that the strong Szegő limit theorem applies. The Fourier coefficients $\hat{c}_k$ are given by

$$\hat{c}_k = \frac{1}{2\pi} \int_0^{2\pi} e^{-ik\theta} \log[1 - 2F(\theta)] d\theta. \quad (39)$$

We can next verify that $\hat{c}_0 = 0$ using symmetries of $\log[1 - 2F(\theta)] = \log|1 - 2F(\theta)| + i\text{Arg}[1 - 2F(\theta)]$. In particular, trigonometric manipulation shows that $\text{Im}[\log f(\theta)] = \text{Im}[\log f(-\theta)]$, $\text{Re}[\log f(\theta)] = \text{Re}[\log f(\pi - \theta)]$, and $\text{Re}[\log f(\theta)] = \text{Re}[\log f(-\theta)]$, which together imply $\hat{c}_0 = 0$. The strong Szegő limit theorem then gives the vison correlator in the $\ell \rightarrow \infty$ limit as the constant

$$\lim_{\ell \rightarrow \infty} |\langle (-1)^{\eta_{E_\ell}} \rangle| = \exp\left(\sum_{k=1}^{\infty} k \hat{c}_{-k} \hat{c}_k\right). \quad (40)$$

The Fourier coefficients $\hat{c}_k$ decay exponentially in $|k|$ since $\log[1 - 2F(\theta)]$ is analytic and $\text{Re}[1 - 2F(\theta)] > 0$. As a result, the sum in Eq. (40) converges, and the limit is nonzero. Evaluating $\hat{c}_k$ and summing over all $|k| \leq 50$ gives

$$\lim_{\ell \rightarrow \infty} |\langle (-1)^{\eta_{E_\ell}} \rangle| = 0.774\,596\,669\dots, \quad (41)$$

which appears to be $\sqrt{60}/10 = 0.774\,596\,669\dots$. We expect an exact evaluation may be possible, for example, using the methods of Ref. [72], which evaluates a more challenging limit. For the purpose of determining the phase, however, it suffices to note that the limit is a nonzero constant, as guaranteed by the convergence of the series in Eq. (40).

We note that calculating spin-spin correlations in the Ising model using Toeplitz determinants goes back to at least Ref. [24], and even an earlier letter in 1950 by Onsager (see for example the introduction in Ref. [70]). In the vison case considered here, we were fortunate that $(\mathcal{K}^{-1})_E(\mathcal{K}')_E$ became exactly a Toeplitz matrix along this particular path. More generally, including for other paths on the square-octagon lattice, $(\mathcal{K}^{-1})_E(\mathcal{K}')_E$ can take the form of a block Toeplitz matrix, to which one may attempt to apply the Szegő–Widom generalization [68,72]. However, in the block case, there is the potential for the limiting coefficient to be zero, in which case the Szegő–Widom theorem need not give any information on the decay rate, though one can in some cases obtain corrections [71]. One instance of the precise calculations needed for the block Toeplitz determinants appears in Ref. [72], which determined the classical monomer-monomer correlations for the triangular lattice dimer model (see the determinant setup of Ref. [31]).

We also note that the oscillating correlations as seen for square path 2 in Fig. 12 can be expressed as determinants of block Toeplitz matrices with alternating *uneven* size blocks, for which evaluating the limit may be more difficult.

E. Nature of the phase

We now interpret the phase of the square-octagon lattice dimer model. Although the dimer-dimer correlator decays exponentially in all directions we considered, the constant vison correlator along certain directions implies that the system is in an ordered phase, not a quantum spin liquid. To understand the nature of the order, we examine the plot of a randomly chosen dimer covering of the square-octagon lattice shown in Fig. 4. We observe that the system does not exhibit one of the typical dimer-ordered phases, such as a staggered or columnar phase. However, this figure reveals key features of the ordering: most of the square plaquettes are flippable, and the diagonal (black) dimers appear only as part of flippable octagon(s). To quantify this latter feature, we compute the conditional probabilities of finding a dimer on various edges, given that there is a dimer on a specific diagonal edge. These conditional probabilities are plotted in Fig. 13. From this figure, one can see that when a diagonal dimer appears, it tends to come in as part of a group of four, all surrounding an octagon face. The exact asymptotic probability can be calculated using the infinite-limit values of $\mathcal{K}^{-1}$ from Eq. (25), combined with the dimer probability formula Eq. (4). Given a diagonal edge e , let P_1 and P_2 be the two adjacent octagon plaquettes. Then we can calculate

$$\mathbb{P}[P_1 \text{ or } P_2 \text{ is flippable} | \text{diag dimer on } e] = 0.9892. \quad (42)$$

Thus, diagonal dimers are accompanied by a flippable octagon face in nearly 99% of the cases.

This gives us the following intuitive picture for the phase of the dimer model: there is a background of flippable

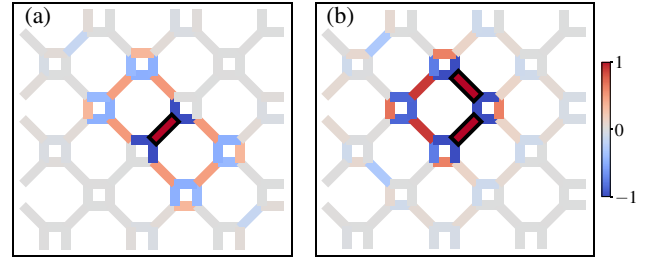


FIG. 13. Change in conditional probabilities, compared to the usual dimer probabilities, for the square-octagon lattice. The color scale corresponds to the scaled difference between the conditional probability and the nonconditional dimer density. The value 1 (dark red) represents the largest possible increase, corresponding to a conditional probability of 1, while -1 (dark blue) represents the largest possible decrease, corresponding to a conditional probability of 0. The value 0, which is gray, represents no change in the conditional probability from the usual (nonconditional) probability of that dimer. From the two plots, we see that a dimer placed on a diagonal edge is very likely to appear as part of a group of four dimers surrounding an octagon face. (a) Change in conditional probabilities given that a dimer occupies the outlined diagonal edge. (b) Change in conditional probabilities given that the two outlined dimers appear on those diagonal edges. This plot shows that the dimers tend to come in a single octagon face, rather than, e.g., a 50% chance of a Fig. 8 shape which would be consistent with (a). The plots are taken in a central region of a radius $R = 50$ region.

square plaquettes, over which there is a finite density of flippable octagonal defects, shown in black in Fig. 4. Such an order is similar to the short range entangled states seen for the Ruby family of Ref. [47] (Sec. V), where different plaquettes are disconnected to from each other. Although in our case on the square-octagon lattice, the square plaquettes are not disconnected, the large number of flippable square plaquettes in Fig. 4 suggests that it has the same order. Using this picture, we can give an intuitive estimate for the vison correlator along the octagon path and the diagonal octagon path shown in Fig. 10, both of which intersect only diagonal edges. Let us label the octagonal plaquettes along the path as $P_0, P_1, P_2, \dots, P_\ell$. Recall that the vison correlator along a path is given by $|p_{\text{odd}} - p_{\text{even}}|$, where p_{odd} and p_{even} are the probabilities that an odd and even number of dimers appear along the path, respectively. Assuming that any diagonal dimer appears only as part of flippable octagon(s), the parity of the number of dimers along the interior octagons $P_1, P_2, \dots, P_{\ell-1}$ will always be even. Let p_{df} denote the probability that an octagonal plaquette is flippable and has dimers along its diagonal edges (we refer to such plaquettes as “diagonal flippable”). The only way to have an odd number of dimers along the vison path is if P_0 is diagonal flippable and P_ℓ is not, or vice versa. Thus,

$$p_{\text{odd}} \approx 2p_{\text{df}}(1 - p_{\text{df}}), \quad (43)$$

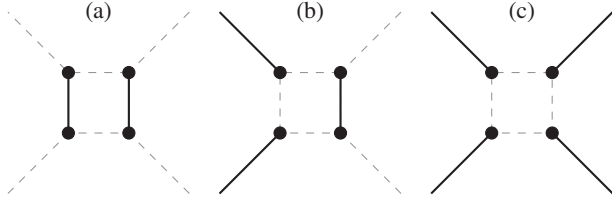


FIG. 14. The three allowed configurations of dimers surrounding a square face (up to rotation and reflection). Subfigures (a), (b), and (c) have zero, two, and four diagonal dimers, respectively, illustrating that the number of diagonal dimers around any square face is always even.

where we use that the edge configurations in P_0 and P_ℓ are nearly independent for large ℓ , since the dimer-dimer correlator decays exponentially. Thus, the vison correlator is $|1 - 2p_{\text{odd}}| \approx |1 - 4p_{\text{df}}(1 - p_{\text{df}})|$. Using Kasteleyn matrix methods, we calculate $p_{\text{df}} = 0.0590$, which gives a vison correlator of 0.7779—in close agreement with the exact analytic result in Eq. (41). Thus, we have shown that the vison correlators along the octagon and diagonal octagon paths are constant, under the assumption that diagonal dimers always appear as part of flippable octagon(s).

From Eq. (42), we see that there is a small probability that the above assumption that diagonal dimers always appear as part of flippable octagons does not hold. One might wonder whether such rare cases could lead to an exponential decay of the vison correlator, albeit with a large correlation length. We argue below why this does not occur. Essentially, when a diagonal dimer does not appear as part of a flippable octagon, it instead participates in a larger flippable loop. To see this, we first note that only three arrangements of diagonal dimers are allowed in the square-octagon lattice by the dimer constraint: no diagonal dimers, dimers extending from two adjacent vertices, or dimers extending from all four vertices, as shown in Fig. 14. If we consider the graph formed solely by the diagonal edges with dimers present—obtained by collapsing each incident square plaquette into a vertex—we see that every interior

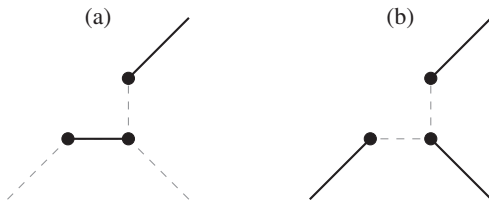


FIG. 15. Allowed configurations of dimers surrounding an inset square in the square-octagon fortress boundary. Unlike interior locations or boundary locations in the rectangular boundary shape, there is an odd number of diagonal dimers surrounding the inset square, causing a chain of diagonal dimers to terminate at this location. Subfigure (a) is responsible for the long chains of diagonal dimers shown in the critical and frozen regions of Fig. 3(a).

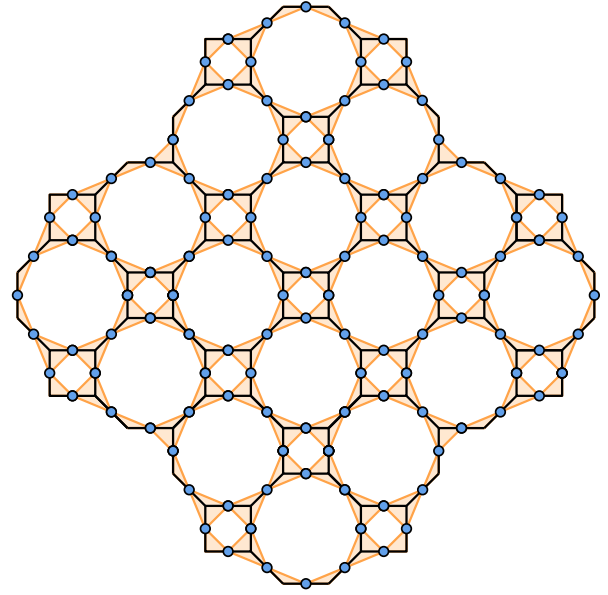


FIG. 16. The figure displays a square-octagon fortress of radius $R = 4$, defined by its black edges. Blue dots indicate the positions of spin-1/2 degrees of freedom. The orange edges represent the line graph of the fortress, forming a graph of corner-sharing polygons.

(non-boundary) vertex in the graph must have even degree. This requirement implies that the collection of diagonal dimers must either form closed loops or extended chains that start and end on the boundary.

In fact, by considering the square or rectangular boundary shown in Figs. 8 and 10, we see in this case the diagonal dimers all occur in loops, with no chains that start or end on the boundary. The same argument above applies to the edges of the region, and the corners, which connect to three diagonal edges, can be analyzed in a similar way to show there must be still be an even number of dimers (zero or two) on those diagonal edges. In contrast, for the fortress boundary shown in Figs. 16 and 17, there are locations in the boundary where chains of diagonal dimers can terminate, specifically at the squares “inset” into the boundary and which lack a protruding corner. These locations, which have three diagonal dimers, have an odd number of diagonal dimers emanating from the inset square as shown in Fig. 15.

It is likely that the probability of finding a flippable chain along a path or loop decays exponentially with the length of the path or loop. In view of this, the earlier assumption that any diagonal dimer appears only as part of a flippable octagon is equivalent to assuming that the only diagonal flippable loops present are the minimal ones surrounding a single octagon face. Now, considering any flippable path of diagonal edges, we can make the following argument: for a diagonal dimer (on edge e) in the bulk of the path to change the parity of the vison string, a diagonal-flippable loop containing e must enclose one of the end points of the path.

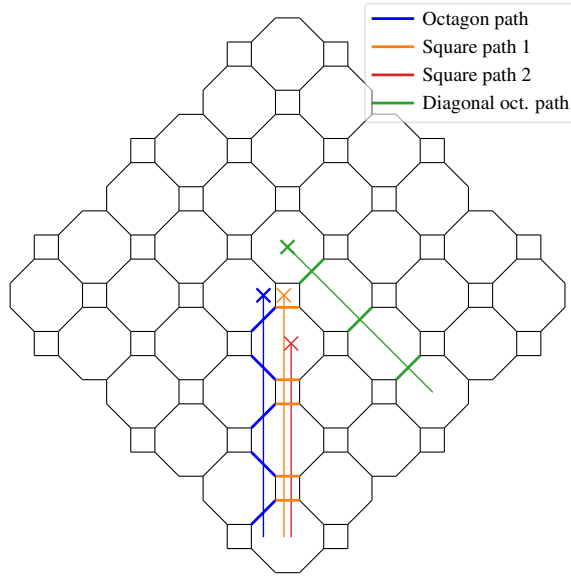


FIG. 17. Paths in the square-octagon fortress with radius $R = 6$ along which we calculate the dimer-dimer and the vison correlators.

Since the probability of a flippable path occurring likely decays at least exponentially with the length of the path, a diagonal dimer on edge e alters the parity of the vison string only with a probability that itself decreases exponentially with the string length. As a result, the vison correlator can still approach a constant in the infinite-length limit. In fact, we expect that if we replace p_{df} in Eq. (43) with the probability

$$p_{\text{o-loops}} \equiv \mathbb{P}[\text{odd\# of diagonal dimer loops around } P] \quad (44)$$

we would obtain an even closer approximation to the analytic vison correlator value in Eq. (41). In summary, our intuitive picture of the dimer model captures certain aspects of its behavior, providing a useful understanding of its underlying structure.

V. PHASE SEPARATION EXAMPLE II: SQUARE-OCTAGON FORTRESS

A. Hamiltonian

In this section, we define the square-octagon fortress graph and the corresponding spin Hamiltonian, whose low-energy limit maps to a quantum dimer model on the square-octagon fortress. The steps are similar to those outlined in Sec. IV A.

The square-octagon fortress is based on the square-octagon lattice described in Sec. IV, but with boundaries rotated by $\pm 45^\circ$ relative to the square-boundary case. Figure 16 shows an example of a square-octagon fortress with radius $R = 4$. Here, the radius is defined as the number of edges crossed by a vertical path extending from the center to infinity. This graph is interesting because it

shows phase separation into three different regions—behavior that appears likely to persist not just at a single fine-tuned point in the phase diagram, but across an extended region.

We begin by explaining the spin and dimer Hamiltonians on the square-octagon fortress, simply called as fortress. In the spin model, the spins are placed on the links of the fortress, as represented by the blue dots in Fig. 16. We then construct the line graph of the fortress and interpret it as a graph of corner-sharing polygons, shaded in orange in the same figure. This line graph helps us define the spin Hamiltonian.

The Hamiltonian of our model on the fortress is symbolically given by Eqs. (19)–(21), with the sums taken over polygons and plaquettes of the fortress, rather than the square-octagon lattice with rectangular boundaries. In the limit $U \gg |V_4|, |V_8|, |J_4|, |J_8|$, we recover an RK quantum dimer model similar to Eq. (22), but now defined on the square-octagon fortress. The ground state of the RK Hamiltonian is the RK wave function on the fortress, which is the uniform superposition of all dimer coverings.

Properties of uniformly sampled dimer coverings on fortress graphs are well studied in the mathematical literature, due to numerical results and their connection to certain weighted versions of the Aztec diamond dimer coverings [7,34,36,37]. Below, we highlight some of these properties and discuss their implications for the phase of both the quantum dimer and spin models.

B. The octic curve

If one uniformly samples dimer coverings of the square-octagon fortress, then it is known, due to numerical results and a well-expected equivalence with a weighted Aztec diamond, that there are three distinct regions as shown in Fig. 3 [7,34,36,37]. The regions near the corners are called the frozen region similar to the frozen region of the dimer coverings of the Aztec diamond. In the frozen region, a random dimer covering will have dimers in a staggered configuration with a probability approaching one in the limit of infinite system size. We can also see from Fig. 3(b) that the average dimer occupation number is (approximately) 0 or 1 for different edges corresponding to the staggered pattern. The innermost region in Fig. 3 is known as the gaseous region in mathematical literature. Finally, the region between the gaseous and the frozen regions is known as the liquid region.

Using coordinates where the fortress boundaries are given by $|x| + |y| = 2$, the boundaries separating these three regions are given by the following “octic (8th-order) curve” [7]:

$$\begin{aligned} &400(x^8 + y^8) + 8025x^4y^4 + 3400(x^2y^6 + y^2x^6) \\ &+ 1000(x^6 + y^6) - 17250(x^4y^2 + x^2y^4) - 1431(x^4 + y^4) \\ &+ 25812x^2y^2 - 3402(x^2 + y^2) + 729 = 0. \end{aligned} \quad (45)$$

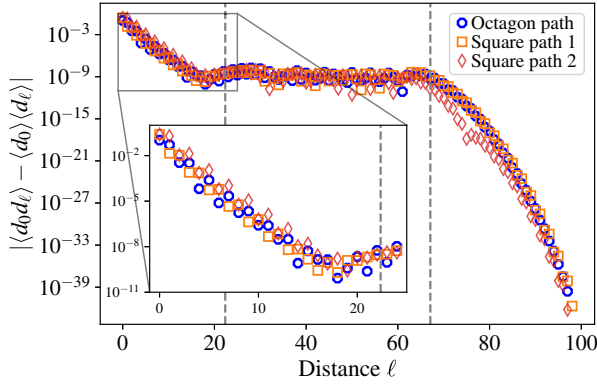


FIG. 18. Log plots of the dimer-dimer correlators along the octagon and the two square paths (depicted in Fig. 17) in the square-octagon fortress, as a function of the edge distance ℓ . Here, recall ℓ is not the Euclidean or graph distance, but is the number of edges between the end points along the path. These correlators were calculated using fraction-free LU decomposition. The correlators show exponential decay in the center phase region (ℓ smaller than around 22 for this fortress), with negatives of the best fit slopes (inverse correlation lengths) between 1.0 and 1.1 as calculated for distances between $\ell = 5$ to 16. This is in close agreement (within ± 0.05) with the dimer correlator for the rectangular boundary square-octagon lattice shown in Fig. 11, as well as its corresponding analytic result 0.774 597.... The fortress for which the correlators are calculated has a radius $R = 100$ and 40 600 vertices. The vertical dashed gray lines show the limiting phase boundary locations according to Eq. (45), which mark changes in the plotted correlators.

This curve is plotted in both parts of Fig. 3, overlaid atop a random dimer configuration in (a) and atop a dimer density plot of the square-octagon fortress in (b). There are two parts of this curve, and they split the fortress into the three distinct regions explained above.

The octic curve formula Eq. (45) was first stated in [7] for diabolo fortress tilings. As explained further in Appendix D, there is also a two-periodic assignment of weights to the Aztec diamond, which makes it “equivalent” to a weighted square-octagon fortress in the sense of sharing certain partition functions and behaviors, such as the Arctic curve and phases [37], which can be obtained from them. A general formula for the Arctic curve of a two-periodic Aztec diamond was given in Sec 3.3 of Ref. [37] in terms of its face weights a , b , c , and d , and specifiable entirely by a single parameter $\alpha = (4/(\frac{a}{b} + \frac{b}{a})(\frac{c}{d} + \frac{d}{c}))^2$. For the unweighted fortress that we consider, the corresponding weighting is given by $a = b = c = 1$ and $d = 1/2$, so that $\alpha = 16/25$ and using that value in Eq. (3.8) of Ref. [37] gives Eq. (45).

C. Dimer-dimer correlator across the phases

The dimer-dimer connected correlator shows distinct behavior in each region of the square-octagon fortress. Using the methods from Sec. II, we numerically calculate

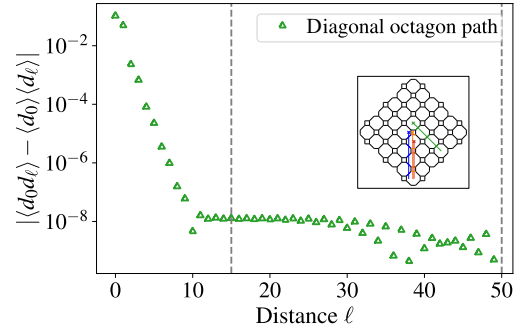


FIG. 19. Log plot of the dimer-dimer connected correlator along the diagonal octagon path as a function of the distance ℓ between the end points. Similar to Fig. 18, the distance is not the Euclidean distance, rather it is the number of edges between the end points along the path. We plot the correlator for the diagonal octagon path here separately from Fig. 18 since the path length and phase boundary locations differ (in particular, this path does not enter a frozen region). The negative of the best fit slope is 1.559 as calculated from $\ell = 3$ to 9, which is similar to that of the rectangular boundary square-octagon lattice shown in Fig. 11.

the dimer-dimer connected correlator and vison correlator along various paths on a square-octagon fortress of radius $R = 100$, where the radius is defined as the number of edges along a horizontal or vertical path from the center to the boundary (including the boundary edge). We evaluate these correlators along the four paths shown in Fig. 17, which are analogous to the paths considered in the square-octagon lattice with rectangular boundaries in Sec. V.

In Fig. 18, we plot the dimer-dimer connected correlator along the octagon path, square path 1, and square path 2 as a function of the edge distance between the end points. The correlator along the diagonal octagon path is shown separately in Fig. 19, since its path length and phase boundary locations differ. For each path, one end point is fixed within the innermost region of the fortress, as indicated by the crosses in Fig. 17. Using Eq. (45) to identify the asymptotic phase boundaries, we observe that the dimer-dimer connected correlator exhibits distinct behaviors across different phases, consistent with expectations. The correlators in the center phase region—covering distances 0 to around 22 along the octagon and square paths—exhibit similar behavior to that of the rectangular-boundary square-octagon lattice shown in Fig. 11. In particular, the dimer-dimer connected correlator decays exponentially, with slopes (i.e., inverse correlation lengths) closely matching those observed in the infinite-size case. In the intermediate critical region, the numerical plots are less conclusive; however, we expect the dimer-dimer connected correlator to exhibit power-law decay as is typical for critical regions. In the frozen regions near the corners, the dimer-dimer connected correlator vanishes in the infinite-size limit, implying that these regions are gapped.

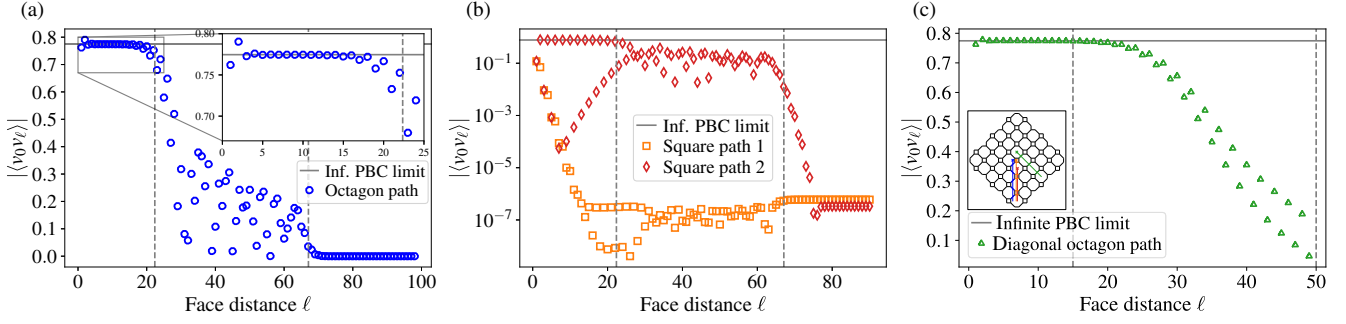


FIG. 20. Vison correlators along the four considered paths [drawn in Fig. 17 and in the inset of (c)] in the square-octagon fortress with radius $R = 100$, calculated using fraction-free LU (FFLU) decomposition. The vertical dashed gray lines show the limiting phase boundaries as before. The vison correlator behavior in the center phase region closely follows that of the rectangular boundary square-octagon lattice shown in Fig. 12. In particular, the octagon and diagonal octagon paths (left-most and right-most plots respectively) show a constant vison correlator in the center phase region. The negative of the best fit slope (inverse correlation length) for the exponential decaying part of square path 1 (orange square marker) is 1.1 as calculated from $\ell = 2$ to 12.

D. Vison correlator across the phases

Now we describe the behavior of the vison correlator along the four paths shown in Fig. 17. Using Eq. (10), we calculate the vison correlators numerically and plot them in Fig. 20. In the central region, the vison correlator along the octagon and diagonal octagon paths approaches a constant for long strings lying entirely within the region. Moreover, this constant matches closely with the analytic value obtained for the square-octagon lattice with rectangular boundaries [Eq. (30)]. In contrast, along square path 1 and square path 2, the vison correlator shows exponential decay with similar correlation lengths or displays oscillating behavior.

In summary, the behavior of both the dimer-dimer connected correlator and the vison correlator in the central region closely matches that on the square-octagon lattice with rectangular boundaries, both qualitatively and quantitatively. This confirms that the central region is in the same phase as the square-octagon lattice with rectangular boundaries, as described in Sec. IV E.

E. Nature of the phase

As in Sec. IV E, it is useful to consider the diagonal dimers to identify the phases, since these paths should be closely related to *height function* [2,73] level lines, which exhibit distinct behavior in different phases (cf. Fig. 2 of Ref. [42]).

We recall the random dimer covering of the square-octagon fortress shown in Fig. 3(a), where diagonal dimers are colored in black. Their behavior is noticeably different across the phases. In the central region, the configuration closely resembles that of the rectangular boundary case in Fig. 4—which is also expected to approximate the infinite-size limit—with diagonal dimers appearing almost exclusively in single-octagon loops. In the intermediate phase, longer and more irregular chains of diagonal dimers begin to emerge. In contrast, the frozen regions consist entirely of

rigidly arranged diagonal dimer chains. In terms of the height function, the center region corresponding to the “smooth or gaseous” phase exhibits minimal fluctuations, with level lines forming only small, localized loops. In the critical or liquid region, it is expected that the height function fluctuations converge, in an appropriate scaling limit, to the Gaussian free field [10,74,75], whose level lines are described by the random fractal curve SLE(4) [76]. In contrast, the frozen phase features a rigid, staggered arrangement, resulting in deterministic level lines for the height function.

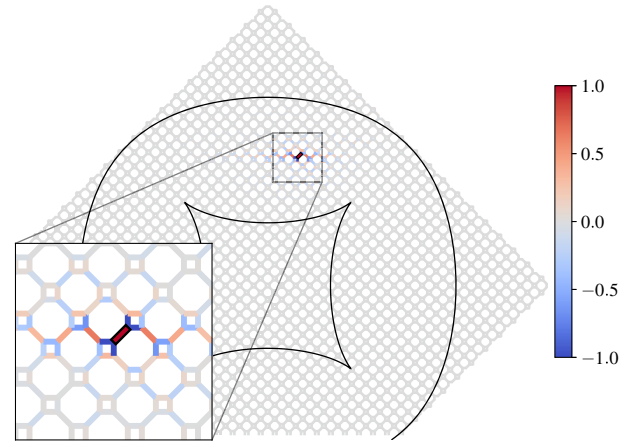


FIG. 21. Conditional probability changes in the critical region of square octagon fortress $R = 40$, using the same color scale as in Fig. 13. As before, the value 0, which is gray, represents no change in the conditional probability from the usual (nonconditional) probability of that particular dimer, while red shows an increase for the conditional probability, and blue shows a decrease for the conditional probability. There is a clear difference here compared to Fig. 13. Instead of coming in a group of four diagonal edges, certain diagonal edges may now form longer horizontal or vertical (depending on location) “strings”.

The contrast between loop and chain configurations is also evident in Fig. 21, which displays the conditional dimer occupation probabilities in the critical region of the square-octagon fortress. Unlike the case of the square-octagon lattice with rectangular boundaries shown in Fig. 13, where diagonal edges tend to form small loops, in the critical region, diagonal dimers more frequently appear as part of extended chains.

VI. DISCUSSION

In this work, we presented two examples of quantum spin and quantum dimer models whose exact ground states have two or three spatially separated phases, challenging standard notions of the thermodynamic limit. Crucially, this phase separation disappears when the same models are placed on domains with differently shaped boundaries. The spin Hamiltonians we consider are defined on graphs of corner-sharing polygons and map to dimer models in their low-energy limit. Our first example is a quantum dimer model defined on the Aztec diamond [2–5]. At the Rokhsar-Kivelson [1] point, we saw that in the ground state, dimers are frozen and have a staggered order in the corner regions outside the Arctic circle [3,5,7,8], while dimers are in a critical phase with power-law decaying dimer-dimer correlators inside the Arctic circle. The inner region resembles the critical dimer phase on the square lattice with rectangular boundaries originally studied by Kasteleyn [21], and Temperley and Fisher [22]. Given the critical correlations inside the Arctic circle, it is likely that the observed phase separation might be fine-tuned to the RK point and would not survive small perturbations away from it. This motivated the second example, a quantum dimer model on the square-octagon lattice. On a square-shaped domain, Kasteleyn methods show that the dimer-dimer correlators decay exponentially with distance along four different paths. To probe if the system is in a quantum spin liquid phase, we numerically calculated the nonlocal vison correlator *exactly* using Kasteleyn-type techniques described in Sec. II B. Along the octagon path, we were also able to calculate the infinite system size and infinite string length limit of the vison correlator analytically, and showed that it approaches a nonzero constant. This implies the system is not in a $\mathbb{Z}_2$ quantum spin liquid phase, rather it is in an ordered phase. We then commented on the order present in the system by considering the diagonal dimers and identified the system to be in a short-range entangled phase. We then studied the same quantum dimer model and corresponding spin Hamiltonian on the square-octagon fortress. Combining numerical calculations of the dimer-dimer and vison correlators with insights from the existing mathematical literature, we showed that at the RK point, the system separates into three distinct phases with different behaviors of the dimer-dimer correlations. The regions near the corners are in an ordered phase with staggered dimers, while the innermost region is in the

same short-range entangled phase as the square-octagon lattice on a square-shaped domain. These regions are separated by a critical region and the boundaries of the three regions are given by the octic curve [7,37]. For the Kasteleyn-based calculations on the fortress, we encounter Kasteleyn matrices with condition numbers growing exponentially in the system size. To get around this issue, we implement fraction-free LU (FFLU) [56–58] decomposition to stably calculate the required inverses. Since the innermost region on the fortress is gapped, we expect that the phase separation persists under small perturbations away from the RK point, likely providing an example of the quantum phase separation extending over a finite region of the phase diagram. We further comment on this below.

We begin with the square lattice with rectangular boundaries. At the RK point this system is critical, and it is known that any generic deviation away from the RK point drives the ground state into an ordered phase [62]. For the Aztec diamond, the region inside the arctic circle is likewise critical at the RK point, and it is therefore natural to expect that a perturbation away from the RK point will also induce ordering within the arctic circle. The fate of phase separation then depends on the nature of the resulting order. If the ordered state in the interior coincides with the staggered order already present in the frozen corners, one would expect the phase separation to disappear, whereas if the interior selects a different ordered state, the phase separation should persist.

We next turn to the square-octagon lattice. With square boundaries, we showed that the RK ground state exhibits exponentially decaying dimer-dimer correlations and realizes a gapped ordered phase, with a nonzero vison correlator indicating vison condensation; because the phase is gapped, it is natural to expect stability under generic small perturbations. With fortress boundaries, we instead find three distinct regions: (i) frozen corners, (ii) an intermediate critical region, and (iii) an inner ordered region that matches the square-boundary ordered phase. The ordering in regions (i) and (iii) is different from each other. The connected dimer-dimer correlator between two points inside the frozen region (i) goes to zero in the infinite-size limit [8,42] implying that the region is gapped. Region (iii) is also gapped due to the exponentially decaying dimer-dimer connected correlator. On the other hand, region (ii) is gapless at the RK point. Upon perturbing away from the RK point, we expect the corners to remain frozen and the visons to be condensed in the central region. Since the orders in regions (i) and (iii) are distinct, we also expect there to be a critical region between the two. Thus, we expect the coexistence of inequivalent bulk phases, each occupying a finite fraction of the system in the thermodynamic limit to persist away from the RK point. A definitive determination of what happens away from the RK point will require further investigation, for

example via quantum Monte Carlo simulations. This will be addressed in a future publication.

Finally, we note that while the RK ground state can be determined exactly, we do not have knowledge of the excited-state spectrum. This prevents a straightforward application of perturbation theory near the RK point, since such an approach would require at least an estimate of the excitation gap together with relevant excited-state matrix elements. Similarly, we also do not know about the thermal stability of the phase separation observed at the RK point. Making quantitative statements at nonzero temperature again requires information about the excitations, which we do not have. Thus, the fate of phase separation at finite temperature therefore remains an open question.

In Sec. II B, we explained a method for calculating the vison correlator exactly and efficiently. This approach applies to general planar graphs and can be used to check if a dimer model on a lattice is in a quantum spin liquid phase at the RK point. Previously, vison correlators were primarily calculated using Monte Carlo methods, and the present method provides a significant advantage in both accuracy and speed. This is particularly valuable for certain lattices with certain boundaries such as the square-octagon fortress, because it is known that the convergence of Monte Carlo simulation with natural ring exchanges is slow [60].

It is often useful to generate a random dimer covering of a lattice. In the mathematics literature, uniform random dimer coverings of the Aztec diamond and the square-octagon fortress are typically generated using the generalized domino shuffling algorithm [4,7], which is efficient and guaranteed to produce a dimer covering drawn uniformly at random. We point out that another method in the literature to produce random dimer coverings is via sampling from determinantal point processes, since Kenyon's formula [Eq. (4)] shows the inverse Kasteleyn matrix essentially gives the correlation kernel for the determinantal point processes formed by the dimers [5,8]. There are efficient methods to generate random samples from such processes [77], which have been applied to generate random samples of tilings of the Aztec diamond. Since this method only requires knowing the inverse Kasteleyn matrix elements, it is easily adaptable to different lattices and boundary shapes. Implementing the determinantal point process sampling algorithm described in Ref. [77], in combination with the fraction-free LU methods from Refs. [56,57] described in Sec. II B, would provide a useful alternative to using Monte Carlo methods to generate random dimer coverings, particularly when the Monte Carlo convergence is slow.

We list below several interesting future directions:

- (1) Identify a lattice which shows phase separation for certain boundary shapes across a finite region of the phase diagram, with at least one region realizing a quantum spin liquid phase.

- (2) Explicitly test the stability of phase separation of the quantum dimer model on the square-octagon fortress [Eq. (22)] away from the RK point using quantum Monte Carlo calculations, which has been used to study several other dimer models [62,78,79].
- (3) The emergence of macroscopic regions with distinct behavior of correlators in dimer models is not unique to the Aztec diamond or the square-octagon fortress; similar phenomena are seen in lozenge tilings of a hexagon [10,80] as well as with Aztec-like boundaries in other bipartite lattices. Investigating the phases of a quantum dimer model corresponding to these different lattices is another compelling direction.
- (4) From an experimental standpoint, Rydberg atom arrays offer a natural platform for realizing dimer models [81–86]. The Rydberg blockade mechanism can be used to impose the dimer constraint on the Kagome lattice [81,82], as well as the square and the triangular lattices [83]. This work has shown that the isotropic Rydberg blockade can be effectively “re-shaped” using vertex *gadgets*, i.e., small auxiliary clusters placed on each lattice vertex, so that excitations on bonds enforce the diluted or fully packed dimer constraint even on lattices where a direct mapping would otherwise fail (e.g., square and triangular geometries) [83]. In this approach, the main experimental knobs are the Rabi drive Ω and detuning Δ on the edge atoms, together with an independently tunable detuning on gadget atoms Δ_{gad} , while the blockade radius is set by the interatomic spacing so as to include all intragadget and vertex-edge distances but exclude further neighbors [83]. Moreover, annealing-type protocols based on ramping $\Omega(t)$ and sweeping the detuning from a large negative value to a positive value were shown numerically to prepare RVB-like equal-weight superpositions of dimer coverings with high fidelity on finite clusters on the square and triangular lattices [83]. These ingredients provide a concrete template for future extensions to the square-octagon lattice, where one would tailor the vertex gadget geometry (and corresponding blockade condition) to enforce the local dimer constraint at each square-octagon vertex, and then tune the resulting effective dimer dynamics toward an RK-type wave function.
- (5) Three-dimensional quantum dimer models are known to exhibit exotic phases, such as a U(1) quantum spin liquid. Dimer models on the simple cubic and diamond lattices have been studied [33,87,88], and it is known that the RK wave function lies in a U(1) quantum spin liquid phase. An interesting question is whether phase separation can occur on a cubic lattice, perhaps with octahedral boundaries, where the regions near the corners may

be in an ordered phase, while region inside a sphere lies in a U(1) spin liquid phase. This would be a three-dimensional analogue of the Aztec diamond and the Arctic circle.

- (6) The method for calculating the vison correlator described in Sec. II B, can be extended to calculate many other important observables, such as the Wilson loops. In particular, the ability to calculate Wilson loops exactly provides a valuable tool for probing confinement or deconfinement in dimer models. Since these quantities decay exponentially with the area or the perimeter, it is crucial to calculate them to a high precision, something which is made possible by the technique in Sec. II B. Using this, we can calculate the expectation value of the Wilson loop operators corresponding to monomers in the RK wave function on the square-octagon fortress for different shapes of the loop. Our preliminary results show that the Wilson loop expectation values follow a perimeter-law or area-law decay depending on the shape of the loop. For the area-law decay, this involves calculating Wilson loop expectation values as small as 10^{-320} . Calculating these extremely small values is possible due to the methods described in Sec. II B. We leave the details for an upcoming work.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data that support the findings of this article are openly available [89,90].

APPENDIX A: KASTELEYN METHOD ON A TORUS

As Kasteleyn showed in Ref. [21], counting dimer configurations on graphs with periodic boundary conditions (PBC) (equivalently, on a torus) requires four distinct Kasteleyn matrices K_n^{00} , K_n^{01} , K_n^{10} , and K_n^{11} . In this section, we write the straightforward generalizations of the dimer-dimer and vison correlator formulas given in Eqs. (6) and (10) to the torus case, which are used in our analytical results. In particular, we verify that in the infinite-size PBC limit, Eqs. (4) and (10) hold with a single inverse function $\mathcal{K}^{-1}$ defined via contour integrals, such as in Eq. (25).

We begin by defining the four Kasteleyn matrices. In what follows, we continue to use the half-size Kasteleyn matrices K_n , defined using the bipartite graph structure, although for non-bipartite graphs, the full-size Kasteleyn matrices $\mathbb{K}_n$ must be used. The periodic graph G_n can be represented as a planar graph PG_n with additional edges connecting the boundary vertices to enforce periodic boundary conditions, thereby realizing the torus topology. These added edges inherit the Kasteleyn orientation from the extended periodic planar graph. The four Kasteleyn matrices $K_n^{\alpha\beta}$ are then defined on PG_n with the usual Kasteleyn weighting, but differ in the weights assigned to the additional edges added to the boundary. For edges (b, w) within PG_n , we have the usual definitions as in the planar case,

$$K_n^{\alpha\beta}(b, w) = \begin{cases} 1, & (b \rightarrow w) \text{ positive orientation} \\ -1, & (b \rightarrow w) \text{ negative orientation} \end{cases}. \quad (\text{A1})$$

However, for the additional edges (b', w') that wrap around the graph to implement the torus topology, the Kasteleyn matrices differ [21]. The first matrix, K_n^{00} , is the simplest to define: it retains the same edge weights as in the planar case, including for the wrap-around edges, using the prescription in Eq. (A1). While this is the most natural extension, it assigns incorrect signs to certain classes of dimer configurations in which dimers wind around the boundaries [21]. To correct for this, the other three matrices K_n^{01} , K_n^{10} , and K_n^{11} modify the signs on the wrap-around edges based on their winding direction. Specifically, for edges (b', w') that wrap around the torus horizontally or vertically, the sign of the edge weight is flipped according to

$$\begin{aligned} K_n^{01}(b', w') &= \begin{cases} K_n^{00}(b', w'), & (b', w') \text{ horizontal} \\ -K_n^{00}(b', w'), & (b', w') \text{ vertical} \end{cases}, \\ K_n^{10}(b', w') &= \begin{cases} -K_n^{00}(b', w'), & (b', w') \text{ horizontal} \\ K_n^{00}(b', w'), & (b', w') \text{ vertical} \end{cases}, \\ K_n^{11}(b', w') &= -K_n^{00}(b', w'). \end{aligned} \quad (\text{A2})$$

In other words, the Kasteleyn matrix $K_n^{\alpha\beta}$ behaves as follows on the additional wrap-around edges: if $\alpha = 1$, it flips the sign of horizontal wrap-around edges, and if $\beta = 1$, it flips the sign of vertical wrap-around edges. Although each individual Kasteleyn matrix $K_n^{\alpha\beta}$ assigns incorrect signs to certain classes of dimer coverings involving dimers crossing the periodic boundary edges, Kasteleyn [21] showed that a linear combination of their Pfaffians yields the correct number of dimer coverings. The number of dimer coverings (i.e., the partition function) on the torus is given by

$$Z_n = \frac{1}{2}(-Z_n^{00} + Z_n^{01} + Z_n^{10} + Z_n^{11}), \quad (\text{A3})$$

where $Z_n^{\alpha\beta} := \det K_n^{\alpha\beta}$ for $\alpha\beta = 00, 01, 10$, and 11 . The relative signs in this expression account for the topological winding sectors and ensure that all dimer configurations are counted exactly once.

Using this counting method, all configurations are accounted for via four determinants instead of a single one. For the dimer-dimer connected correlator $C_{\mu\nu}^d$ between two edges $\mu = (b_1, w_1)$ and $\nu = (b_2, w_2)$, we have [64, §8],

$$\begin{aligned} C_{\mu\nu}^d &= \langle d_\mu d_\nu \rangle - \langle d_\mu \rangle \langle d_\nu \rangle \\ &= \frac{\sum_{\alpha\beta} \varepsilon_{\alpha\beta} |(K_n^{\alpha\beta})^{-1}(w_2, b_1)(K_n^{\alpha\beta})^{-1}(w_1, b_2)| \det [K_n^{\alpha\beta}]}{\sum_{\alpha\beta} \varepsilon_{\alpha\beta} \det [K_n^{\alpha\beta}]}, \end{aligned} \quad (\text{A4})$$

where $\varepsilon_{00} = -1$, $\varepsilon_{\alpha\beta} = 1$ for the other three combinations of $\alpha\beta \in \{01, 10, 11\}$.

In the infinite-size limit $n \rightarrow \infty$, it is known (or can be verified) that the matrix elements $(K^{\alpha\beta})^{-1}(w, b)$ converge (at least along a subsequence, in the case of critical behavior) to a common limiting function $\mathcal{K}^{-1}(w, b)$, given by a contour integral representation [42, §4], such as that in Eq. (25). This yields a simple expression for the dimer-dimer connected correlator in the infinite-volume limit (in the uniform edge weight or unweighted case, which includes all the graphs in the main text):

$$|C_{\mu\nu}^d| = |\mathcal{K}^{-1}(w_2, b_1)\mathcal{K}^{-1}(w_1, b_2)|. \quad (\text{A5})$$

For the vison correlator, we have

$$\langle (-1)^{\eta_E} \rangle = \frac{\sum_{\alpha\beta} \varepsilon_{\alpha\beta} \det \tilde{K}_n^{\alpha\beta}}{\sum_{\alpha\beta} \varepsilon_{\alpha\beta} \det K_n^{\alpha\beta}}, \quad (\text{A6})$$

where $\tilde{K}_n^{\alpha\beta} = K_n^{\alpha\beta} - (K_n^{\alpha\beta})'$, and the matrices $\tilde{K}_n^{\alpha\beta}$ and $(K_n^{\alpha\beta})'$ are defined as in Sec. II B. Using the block structure of $(K_n^{\alpha\beta})'$ and denoting by $(\cdot)_E$ the restriction to the $\ell \times \ell$ submatrix associated with the string E , we obtain

$$\langle (-1)^{\eta_E} \rangle = \frac{\sum_{\alpha\beta} \varepsilon_{\alpha\beta} \det [K_n^{\alpha\beta}] \det [I_\ell - (K_n^{\alpha\beta})'_E ((K_n^{\alpha\beta})^{-1})_E]}{\sum_{\alpha\beta} \varepsilon_{\alpha\beta} \det [K_n^{\alpha\beta}]}, \quad (\text{A7})$$

where the sum is over the four values of $\alpha\beta$, $\varepsilon_{00} = -1$, and $\varepsilon_{\alpha\beta} = +1$ for the other three $\alpha\beta$. If the string E does not wrap around the torus, as will be the case since we consider a finite-length string in the infinite-size limit, then all four matrices $(K_n^{\alpha\beta})'_E$ are identical. In the limit $n \rightarrow \infty$, as before we know the matrix elements

$(K^{\alpha\beta})^{-1}(w, b)$ all converge to the same value $\mathcal{K}^{-1}(w, b)$ given by contour integrals. Consequently, all determinants $\det [I_\ell - (K_n^{\alpha\beta})'_E ((K_n^{\alpha\beta})^{-1})_E]$ converge to the same value $\det [I_\ell - (\mathcal{K}')_E (\mathcal{K}^{-1})_E]$, and Eq. (A7) becomes

$$\langle (-1)^{\eta_E} \rangle = \det [I_\ell - (\mathcal{K}')_E (\mathcal{K}^{-1})_E]. \quad (\text{A8})$$

APPENDIX B: KASTELEYN DERIVATION FOR THE INFINITE SQUARE-OCTAGON LATTICE

In this section we provide the details for deriving Eq. (25), which gives the matrix elements of the inverse of the Kasteleyn matrix for an square-octagon lattice on an infinite torus.

1. Full-size Kasteleyn matrices

For this derivation, we primarily work with the full-size Kasteleyn matrices $\mathbb{K}_n^{00}, \mathbb{K}_n^{01}, \mathbb{K}_n^{10}$, and $\mathbb{K}_n^{11}$, both for convenience and to better follow along with the method in Ref. [64]. These are the same type of matrices used when working with nonbipartite planar graphs. Instead of starting with the half-size adjacency matrix A , whose rows are indexed by vertices in B and columns by vertices in W , we consider the full-size $2N \times 2N$ adjacency matrix $\mathbb{A}$, with both rows and columns indexed by the full set of vertices V . The entries of $\mathbb{A}$ are defined as $\mathbb{A}(v_i, v_j) = 1$ if the vertices v_i and v_j are connected by an edge, and 0 otherwise. Similarly, we define a full-size $2N \times 2N$ signed adjacency matrix (i.e., the Kasteleyn matrix) $\mathbb{K}$ in the same way as before, using the Kasteleyn weighting and Eq. (3), applied to all vertex pairs (v_i, v_j) . Kasteleyn [48, 49] showed that the number of dimer coverings is given by the *Pfaffian* of the skew-symmetric matrix $\mathbb{K}$:

$$\begin{aligned} \text{No.}\{\text{dimer coverings}\} &= |Pf(\mathbb{K})| \\ &= \frac{1}{2^N N!} \left| \sum_{\sigma \in S_{2N}} \text{sgn}(\sigma) \prod_{i=1}^N \mathbb{K}(\sigma(2i-1), \sigma(2i)) \right|. \end{aligned} \quad (\text{B1})$$

For any skew-symmetric $\mathbb{K}$, we have the identity $|Pf(\mathbb{K})| = \sqrt{\det \mathbb{K}}$, so the number of dimer coverings can equivalently be expressed in terms of the determinant.

In the case where the graph G is bipartite, indexing the vertices such that all black vertices B precede the white vertices W gives the large Kasteleyn matrix $\mathbb{K}$ the block structure

$$\mathbb{K} = \begin{pmatrix} 0 & K \\ -K^\dagger & 0 \end{pmatrix}, \quad (\text{B2})$$

where K denotes the half-size Kasteleyn matrix. Throughout, we use K to refer to this smaller half-size

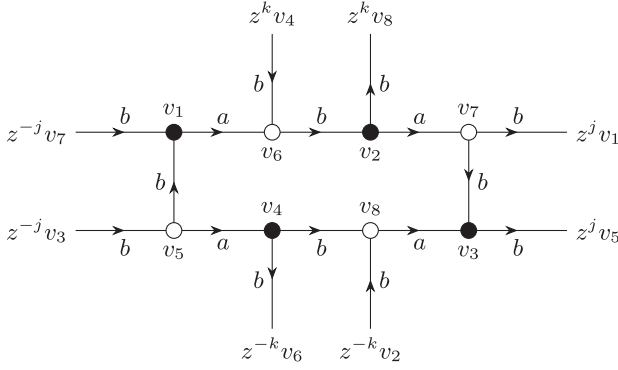


FIG. 22. Fundamental cell of the square-octagon lattice, drawn as a subgraph of a square lattice by “flattening” the octagons. Values of a vector in the z^j eigenspace of $T_{(4,0)}$ and the z^k eigenspace of $T_{(0,2)}$. The vector is determined by its values $v_1, \dots, v_8$ in a fundamental domain.

Kasteleyn matrix and reserve the notation $\mathbb{K}$ for the “large-size” Kasteleyn matrix. With this block structure, the Pfaffian and determinant are related by $Pf(\mathbb{K})^2 = \det \mathbb{K} = |\det K|^2$, thereby recovering the determinant formula Eq. (2) for bipartite graphs. Note that in this formulation, the matrix K has rows indexed by black vertices b_i and columns indexed by white vertices w_i , so the inverse matrix K^{-1} has rows indexed by w_i and columns by b_i .

2. Square-octagon partition function

Because it can be useful for calculating quantities such as edge probabilities, we place edge weights a on the octagon (nonsquare) edges and b on the square edges, as depicted in Fig. 22. Ultimately, we will set $a = b = 1$ to recover the uniform (unweighted) case studied in the main text. To clarify the horizontal and vertical translation of fundamental cells, we depict the octagons in a compressed form in Fig. 22, allowing the lattice to be viewed as a subset of $\mathbb{Z}^2$. Recall that G_n denotes the PBC graph formed by applying n horizontal and n vertical translations of the fundamental cell. Viewed as a subset of $\mathbb{Z}^2$, it is a $2n \times 4n$ (height $\times$ width) subset of $\mathbb{Z}^2$ with edges kept according to the square-octagon lattice pattern. The partition function Z_n with edge weights a and b is defined as

$$Z_n = \sum_{\{\text{dimer coverings}\}} a^{N_a} b^{N_b},$$

where N_a and N_b denote the number of dimers on edges with weights a and b , respectively, in each dimer covering.

Recall we will primarily work with the large Kasteleyn matrices $\mathbb{K}_n^{00}, \mathbb{K}_n^{01}, \mathbb{K}_n^{10}$, and $\mathbb{K}_n^{11}$, for convenience and to better follow along with the method in Ref. [64]. These matrices are skew symmetric, satisfying $(\mathbb{K}_n^{\alpha\beta})^\dagger = -\mathbb{K}_n^{\alpha\beta}$, and have the block structure written in Eq. (B2), with the

$\mathbb{K}_n^{\alpha\beta}$ defined in Appendix A. These full-size matrices each have dimensions $(8n^2) \times (8n^2)$, with rows and columns indexed by all vertices of the graph G_n . Although complex phases are sometimes used in defining Kasteleyn matrices, we restrict ourselves to real phases (such as signs), since this is important for numerical calculations involving exact integer arithmetic.

Recall that we label each vertex in G_n by coordinates (x, y, t) , where (x, y) denotes the fundamental cell translation, and $t \in \{1, \dots, 8\}$ specifies the internal vertex label within the cell, corresponding to positions $v_1, \dots, v_8$. With this indexing, the matrix $\mathbb{K}_n^{00}$ is given by

$$\begin{aligned} \langle x, y, t | \mathbb{K}_n^{00} | j, k, s \rangle &= \begin{cases} \varepsilon_e a, & e = ((x, y, t) \rightarrow (j, k, s)) \text{ has weight } a \\ \varepsilon_e b, & e = ((x, y, t) \rightarrow (j, k, s)) \text{ has weight } b, \\ 0, & ((x, y, t) \rightarrow (j, k, s)) \text{ is not an edge} \end{cases} \end{aligned} \quad (\text{B3})$$

where the orientation $\varepsilon_e \in \{\pm 1\}$ of an edge e is defined to be $+1$ if it agrees with the Kasteleyn orientation (i.e., the arrow directions) indicated in Figs. 9 and 22, and -1 if it opposes it. The other matrices $\mathbb{K}_n^{\alpha\beta}$ are defined analogously, except that the signs are flipped on certain edges that wrap around the torus, as described earlier in Appendix A. Then we have [21]

$$\begin{aligned} Z_n &= \frac{1}{2} \left(-\sqrt{\det \mathbb{K}_n^{00}} + \sqrt{\det \mathbb{K}_n^{01}} \right. \\ &\quad \left. + \sqrt{\det \mathbb{K}_n^{10}} + \sqrt{\det \mathbb{K}_n^{11}} \right). \end{aligned} \quad (\text{B4})$$

To compute $\det \mathbb{K}_n^{\alpha\beta}$ and $(\mathbb{K}_n^{\alpha\beta})^{-1}$, we block diagonalize the matrices $\mathbb{K}_n^{\alpha\beta}$ using a Fourier transform, following for example the method in Sec. 7 of Ref. [64]. For brevity, we provide full details only for the $\mathbb{K}_n^{00}$ case, since as discussed in Refs. [64, 42], it can be verified that the entries of $(\mathbb{K}_n^{\alpha\beta})^{-1}$ converge, in the infinite-size limit, to the same contour integral expressions for all choices of $\alpha\beta$. The matrix $\mathbb{K}_n^{00}$ is especially convenient to work with since it commutes with the translation operators $T_{(4,0)}$ and $T_{(0,2)}$, where $T_{(m,n)}$ denotes a shift in the x direction by m and in the y direction by n . The translation operator $T_{(4,0)}$ is a shift by one fundamental domain in the x direction, while $T_{(0,2)}$ is a shift by one fundamental domain in the y direction. The eigenspaces of these shift operators can be easily determined. Since $T_{(4,0)}^n = I$ and $T_{(0,2)}^n = I$, the eigenvalues of these operators are n th roots of unity, i.e., powers of $z := e^{2\pi i/n}$. For a fixed eigenvalue z^j of $T_{(4,0)}$, the corresponding eigenspace has dimension $4(2n) = 8n$, and an eigenvector is determined by its values on four adjacent columns, which each have length $2n$. Similarly, for an eigenvalue z^k of $T_{(0,2)}$, the eigenspace has dimension $8n$

and an eigenvector is determined by its values on two adjacent rows, which each have length $4n$. A vector in the z^j eigenspace of $T_{(4,0)}$ and the z^k eigenspace of $T_{(0,2)}$ is fully determined by its values in a 2×4 block of the lattice, which can be taken to be a fundamental domain.

Following Ref. [64], define the vector $e_{j,k}^{(s)}$ by

$$\langle x, y, t | e_{j,k}^{(s)} \rangle = \frac{1}{n} \begin{cases} z^{jx+ky}, & t = s \\ 0, & \text{otherwise} \end{cases}.$$

The vector $e_{j,k}^{(s)}$ is a z^j eigenvector of $T_{(4,0)}$ and a z^k -eigenvector of $T_{(0,2)}$. It selects a single vertex s in a fundamental domain and translates it across all of G_n , with the appropriate eigenvalue prefactors. Since there are n^2 translates of a fundamental domain vertex s [one for each (x, y)], the vector $e_{j,k}^{(s)}$ is properly normalized (in ℓ^2 norm). Let S be the $8n^2 \times 8n^2$ matrix whose columns are the $e_{j,k}^{(s)}$ for $s \in \{1, \dots, 8\}$ and $(j, k) \in \{0, \dots, n-1\}^2$, ordered so that vectors with the same (j, k) appear consecutively,

$$(e_{jk}^{(1)}, \dots, e_{jk}^{(8)})_{jk}.$$

One can verify that S is unitary, and that it block-diagonalizes $\mathbb{K}_n^{00}$ as follows:

$$S^{-1} \mathbb{K}_n^{00} S = \begin{pmatrix} B_{0,0} & & & \\ & B_{0,1} & & \\ & & \ddots & \\ & & & B_{n-1,n-1} \end{pmatrix}, \quad (\text{B5})$$

where each block

$$B_{j,k} = \begin{pmatrix} 0 & B_{jk,1} \\ -B_{jk,1}^\dagger & 0 \end{pmatrix} \quad (\text{B6})$$

is an 8×8 matrix, indexed by the vertex labels $v_1, \dots, v_8$ as shown in Fig. 22, and describes the action of $\mathbb{K}_n^{00}$ on the intersection of the z^j eigenspace of $T_{(4,0)}$ and the z^k eigenspace of $T_{(0,2)}$.

Using Fig. 22, we see that

$$B_{jk,1} = \begin{pmatrix} -b & a & -bz^{-j} & 0 \\ 0 & -b & a & bz^k \\ bz^j & 0 & -b & -a \\ -a & bz^{-k} & 0 & b \end{pmatrix}. \quad (\text{B7})$$

Because of the block-diagonal structure of $S^{-1} \mathbb{K}_n^{00} S$, we obtain the determinant of $\mathbb{K}_n^{00}$ as the product

$$\begin{aligned} \det \mathbb{K}_n^{00} &= \prod_{j,k=0}^{n-1} |\det B_{jk,1}|^2 \\ &= \prod_{j,k=0}^{n-1} |-a^4 - 4b^4 + a^2 b^2 (z^j + z^{-j} + z^k + z^{-k})|^2, \end{aligned} \quad (\text{B8})$$

where $z = e^{2\pi i/n}$. Recall that the full partition function Z_n involves a linear combination of four such determinants, as in Eq. (24). The formulas for the other three Kasteleyn-type matrices are similar, though they may commute with a composition of a translation and negation of certain entries, rather than just the translations. In the $n \rightarrow \infty$ limit all quantities we are interested in will be the same for any of the four terms [42,64].

Taking a logarithm or derivative of $\sqrt{\det \mathbb{K}_n^{00}}$ converts the product over j, k in Eq. (B8) into a sum over j, k . In the limit $n \rightarrow \infty$, the discrete sums over j and k become Riemann sums, which approximate double integrals over the torus. Specifically, terms involving $z^j = e^{2\pi i j/n}$ are replaced by continuous variables $e^{2\pi i t}$ for $t \in [0, 1)$, leading to contour integrals or integrals over the torus $[0, 1)^2$ in the thermodynamic limit. For example, in the uniform case $a = b = 1$, we have

$$Z_n^{\alpha\beta} = \prod_{z^n=(-1)^\alpha} \prod_{w^n=(-1)^\beta} (-5 + z + z^{-1} + w + w^{-1}), \quad (\text{B9})$$

where the products are taken over n th roots of unity z and w satisfying the appropriate twisted boundary conditions determined by $\alpha\beta$. Using a Riemann sum approximation, this product becomes a double integral in the limit $n \rightarrow \infty$, yielding the limiting free energy per unit cell:

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{1}{n^2} \log Z_n \\ = \frac{1}{(2\pi i)^2} \oint_{S^1} \frac{dz}{z} \oint_{S^1} \frac{dw}{w} \log |-5 + z + z^{-1} + w + w^{-1}|. \end{aligned} \quad (\text{B10})$$

The function $P(z, w) = -5 + z + z^{-1} + w + w^{-1}$ is known as the *characteristic polynomial* of the graph [42]. It can be easily calculated from the fundamental cell and determines many key properties of the model, including whether the dimer-dimer correlators have exponential decay or power-law decay [42].

3. Dimer occupation probabilities

In the limit $n \rightarrow \infty$, the above calculations give the expected dimer occupation number on the diagonal edges (edges with weight a in Fig. 22) as

$$\begin{aligned}\mathbb{E}[e_a] &= \lim_{n \rightarrow \infty} \frac{a}{4n^2 Z_n} \frac{\partial Z_n}{\partial a} \\ &= \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{-a^4 + a^2 b^2 (\cos t + \cos s)}{-a^4 - 4b^4 + 2a^2 b^2 (\cos t + \cos s)} dt ds.\end{aligned}\quad (\text{B11})$$

For uniform edge weights $a = b = 1$, this simplifies to

$$\begin{aligned}\mathbb{E}[e_a] &= \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{-1 + \cos t + \cos s}{-5 + 2(\cos t + \cos s)} dt ds \\ &= 0.118925 \quad (\text{to six decimal places}).\end{aligned}\quad (\text{B12})$$

The expected dimer occupation number for the square edges (edges with weight b in Fig. 22) is then

$$\mathbb{E}[e_b] = \frac{1 - \mathbb{E}[e_a]}{2} = 0.440537 \quad (\text{to six decimal places}).\quad (\text{B13})$$

4. Inverse Kasteleyn matrix

To determine the entries of the inverse Kasteleyn matrix, we return to the block-diagonal form of $S^{-1} \mathbb{K}_n^{00} S$ as described in Eq. (B5). Taking the inverse yields

$$(\mathbb{K}_n^{00})^{-1} = S \begin{pmatrix} B_{0,0}^{-1} & & & \\ & B_{0,1}^{-1} & & \\ & & \ddots & \\ & & & B_{n-1,n-1}^{-1} \end{pmatrix} S^{-1}, \quad (\text{B14})$$

where each B_{jk}^{-1} has the block form

$$B_{jk}^{-1} = \begin{pmatrix} 0 & (-B_{jk,1}^\dagger)^{-1} \\ B_{jk,1}^{-1} & 0 \end{pmatrix}, \quad (\text{B15})$$

where $B_{jk,1}$ is defined in Eq. (B7). The inverse of $B_{jk,1}$ can be explicitly calculated as

$$\begin{aligned}B_{jk,1}^{-1} &= \frac{1}{-a^4 - 4b^4 + a^2 b^2 (z^j + z^{-j} + z^k + z^{-k})} \\ &\times \begin{pmatrix} 2b^3 - a^2 b z^{-k} & ab^2 - ab^2 z^{-j-k} & a^2 b - 2b^3 z^{-j} & a^3 - ab^2 z^{-j} - ab^2 z^k \\ -a^3 + ab^2 z^j + ab^2 z^k & 2b^3 - a^2 b z^{-j} & ab^2 - ab^2 z^{k-j} & a^2 b - 2b^3 z^k \\ 2b^3 z^j - a^2 b & -a^3 + ab^2 z^j + ab^2 z^{-k} & 2b^3 - a^2 b z^k & ab^2 - ab^2 z^{j+k} \\ ab^2 - ab^2 z^{j-k} & a^2 b - 2b^3 z^{-k} & a^3 - ab^2 z^{-j} - ab^2 z^{-k} & a^2 b z^j - 2b^3 \end{pmatrix}.\end{aligned}\quad (\text{B16})$$

Noting that $\langle w, z, s | S | j, k, t \rangle = e^{2\pi i(jw+kz)} \delta_{t,s}/n$, we obtain the inverse matrix entries as

$$\langle w, z, s | (\mathbb{K}_n^{00})^{-1} | x, y, t \rangle = \sum_{j,k=0}^{n-1} \frac{1}{n^2} e^{2\pi i(jw+jz)/n} e^{-2\pi i(jx+ky)/n} \langle t | B_{jk}^{-1} | s \rangle. \quad (\text{B17})$$

Similar formulas apply to the other matrices $\mathbb{K}^{\alpha\beta}$ for $\alpha\beta = 01, 10, 00$. In the limit $n \rightarrow \infty$, the entries of all $\mathbb{K}_n^{\alpha\beta}$ converge to the same contour integral expressions [42] (Sec. S4) via a Riemann sum approximation. With $2\pi i j/n$ and $2\pi i k/n$ becoming the continuous variables k_x and k_y , respectively, this yields Eq. (25). The expressions in Eq. (26) are just the entries of $B_{jk,1}^{-1}$ in the special case $a = b = 1$ and without the prefactor $1/P(z, w)$. Note that for Eq. (26), we determine the row and column indices of the table and of $B_{jk,1}^{-1}$ by looking at its placement in the block structure of the larger skew-symmetric matrix B_{jk}^{-1} in Eq. (B15), which has rows and columns indexed by $1, 2, \dots, 8$.

To simplify the double integrals appearing in Eq. (25), we consider the following transformation for generic $j, k \in \mathbb{Z}$:

$$\begin{aligned}\frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{e^{ij\theta} e^{ik\phi}}{-5 + 2\cos\theta + 2\cos\phi} d\theta d\phi &= \frac{1}{(2\pi i)^2} \oint_{S^1} \oint_{S^1} \frac{z^j w^k}{-5 + z + z^{-1} + w + w^{-1}} \frac{dz dw}{z w} \\ &= \frac{1}{(2\pi i)^2} \oint_{S^1} \frac{z^j dz}{z} \oint_{S^1} \frac{w^k dw}{[w - \alpha(z)][w - \beta(z)]},\end{aligned}\quad (\text{B18})$$

where the functions $\alpha(z)$ and $\beta(z)$ are given by

$$\alpha(z), \beta(z) = \frac{1}{2} \left(5 - z^{-1} - z \mp \sqrt{(-5 + z^{-1} + z)^2 - 4} \right). \quad (\text{B19})$$

For $|z| = 1$, the functions $\alpha(z)$ and $\beta(z)$ are real valued, and one can verify that $|\alpha(z)| < 1$ and $|\beta(z)| > 1$. Therefore, in the contour integral Eq. (B18), if $k \geq 0$, the only pole inside the unit circle is at $w = \alpha(z)$, giving the single-residue contribution:

$$\begin{aligned} & \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{e^{ij\theta} e^{i|k|\phi}}{-5 + 2\cos\theta + 2\cos\phi} d\theta d\phi \\ &= \frac{1}{2\pi i} \oint_{S^1} \frac{z^j \alpha(z)^{|k|} dz}{z[\alpha(z) - \beta(z)]} \\ &= -\frac{1}{2\pi} \int_0^{2\pi} \frac{e^{ij\theta} \left[\frac{1}{2}(5 - 2\cos\theta - \sqrt{(5 - 2\cos\theta)^2 - 4}) \right]^{|k|}}{\sqrt{(5 - 2\cos\theta)^2 - 4}} d\theta. \end{aligned} \quad (\text{B20})$$

If $k < 0$ in the integral on the left-hand side of Eq. (B18), we can first substitute $\phi \mapsto -\phi$ in the starting integral of Eq. (B20) to take $k > 0$. Note this agrees intuitively, since in an infinite-size limit or on a torus it is symmetric to shift the fundamental cell by k or $-k$.

APPENDIX C: NUMERICAL DETAILS

In this section, we briefly discuss numerical details specific to the Aztec diamond and the square-octagon fortress. In contrast to the square or square-octagon lattices with square boundary conditions, it turns out that the Kasteleyn matrices for the Aztec diamond and square-octagon fortress have large condition numbers $\kappa := \|K\| \|K^{-1}\|$, which may exceed 10^{16} even for small system sizes (see Fig. 23). This implies that standard inversion techniques and LU decomposition are numerically unreliable: for every power of 10 in the condition number, one may lose roughly that many digits of precision when solving linear systems [91]. In practice, attempting to use the standard floating point LU decomposition can give vison correlator values greater than one which is impossible and indicates numerical inaccuracies. Similarly, using floating point LU to calculate dimer densities for large fortresses can give clear inaccuracies and non-symmetric values despite the horizontal and vertical reflection symmetries of the fortress. Numerical instabilities involving K^{-1} for the Aztec diamond were also observed in Ref. [77].

To circumvent these issues, we implement a fraction-free LU decomposition as described in Sec. II B, based on the sparse version of the Bareiss algorithm introduced in Ref. [56] (see also Ref. [57]). Although our implementation is significantly slower than standard floating point LU methods, it uses exact integer arithmetic—handling integers of magnitude $> 10^{1700}$ for the plots in

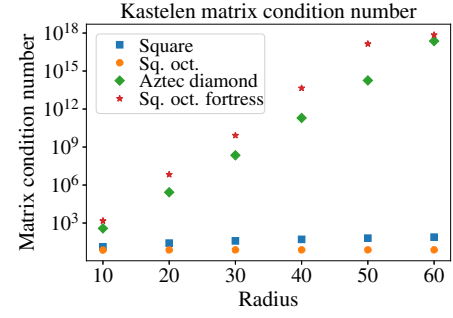


FIG. 23. Condition number of the Kasteleyn matrices for four models as a function of the system size. While the square boundary condition Kasteleyn matrices have a very small condition number (of order 10^1 or 10^2 in the plot), the Aztec diamond and fortress boundary conditions lead to exponentially large condition numbers, indicating that the standard floating point LU or determinant calculations can be entirely inaccurate for these matrices.

Sec. V—and produces the exact rational values of the submatrix $(K^{-1})_E$.

APPENDIX D: CORRESPONDENCE BETWEEN LATTICES

Here, we explain briefly the correspondence between the weighted Aztec diamond and the square-octagon fortress. It is well established in the mathematical literature that the unweighted square-octagon fortress corresponds to a particular assignment of edge weights of the Aztec diamond [7,37].

While we consider the fortress with uniform weights since it can be formulated clearly in terms of spin Hamiltonians, many results in the mathematical literature deal with the weighted Aztec diamond model instead. The T -system procedure, described in Ref. [37], establishes an equivalence between various weighted Aztec diamonds and weighted square-octagon fortresses. The correspondence holds up to general patterns of *face* weighting, where each face F is assigned a weight W_F . This induces an edge weight w_e for each edge e given by the product of the face weights of the two faces adjoining the edge e . Note that while all face weightings are edge weightings, the converse is not true. The partition function for the Aztec diamond of radius k is given in terms of face weights W_f , and in terms of edge weights w_e :

$$\begin{aligned} Z_k &= \sum_{\text{configs}} \prod_{\text{faces } f} (W_f)^{D_f - 1} \\ &= \left(\prod_{\text{faces } f} \frac{1}{W_f} \right) \sum_{\text{configs}} \prod_{\text{edges } e} (w_e)^{D_e}, \end{aligned} \quad (\text{D1})$$

where D_f is the sum of the dimer occupation numbers of the four edges surrounding a face f , and D_e is the dimer occupation number of a single edge e .

For the square-octagon fortress, the definition of the partition function has to be modified compared to the simple square lattice, due to faces having different numbers of edges surrounding them:

$$Z_k = \sum_{\text{configs}} \prod_{\text{faces } f} (W_f)^{D_f + 1 - \frac{v_f}{2}} = \left(\prod_{\text{faces } f} W_f^{1 - \frac{v_f}{2}} \right) \sum_{\text{configs}} \prod_{\text{edges } e} (w_e)^{D_e}, \quad (\text{D2})$$

where v_f represents the number of vertices (4 or 8) surrounding the face designated f , and w_e is defined in the same way it was previously.

The correspondence provides, in our case, a set of face weights on the square Aztec diamond whose Arctic curves [37] and whose partition function are identical to that of a square-octagon fortress with another set of weights. Details of the process for obtaining this correspondence are given in Ref. [92], where the square-octagon lattice is considered a particular case of a more general type of lattice consisting of square, hexagon, and octagon plaquettes. The method treats these lattices as an alteration of the basic square grid, such that the correspondence between plaquettes is one-to-one. In this case, the alteration contracts the four octagon-octagon edges emanating from each square into single points.

We will only state the relevant final results here. For a square-octagon fortress where we assign a face weight w_s to all squares and a face weight 1 to all octagons, or equivalently, a weight of 1 to all diagonal edges and a weight of w_s to all horizontal and vertical edges, the corresponding face weights for the Aztec diamond that has the same partition function and same Arctic curve are given as

$$\begin{cases} W_{i,j} = 1, & i + j \equiv 1 \pmod{2} \\ W_{i,j} = w_s, & i \equiv 0 \pmod{2}, j \equiv 0 \pmod{2} \\ W_{i,j} = \frac{1}{2w_s}, & i \equiv 1 \pmod{2}, j \equiv 1 \pmod{2}, \end{cases} \quad (\text{D3})$$

where (i, j) represent coordinates on a two-dimensional grid that are assigned to each face. Since these weights depend only on the faces' coordinates modulo 2, this weight assignment is called "2-periodic." The weights of faces are conventionally denoted by a, b, c, d whose coordinates are (even, odd), (odd, even), (even, even), and (odd, odd) respectively. These parameters are employed in the formula [37] (Sec. III. 3) for the Arctic octic curve (as used in Sec. VB) of the square-octagon fortress, and additional formulas for properties of the weighted Aztec diamond.

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