Finite-size scaling and boundary effects in two-dimensional valence-bond-solids

Anders W. Sandvik
Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215, USA

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Various lattice geometries and boundary conditions are used to investigate valence-bond-solid (VBS) ordering in the ground state of an $S = 1/2$ square-lattice quantum spin model—the $J$-$Q$ model, in which four- or six-spin interactions $Q$ are added to the standard Heisenberg exchange $J$. Ground state results for finite systems (with up to thousands of spins) are obtained using an unbiased projector quantum Monte Carlo method. It is found that great care has to be taken when extrapolating the order parameter to infinite lattice size, in particular in cylinder geometry. Even though strong VBS order exists in two dimensions, and is established clearly with increasing system size on $L \times L$ lattices (or $L_x \times L_y$ lattices with a fixed aspect ratio $L_x/L_y$ of order 1), only short-range VBS correlations are observed on long cylinders (when $L_x \to \infty$ at fixed $L_y$). The correlation length increases with the cylinder width, until long-range order sets in at a “critical” width. This width is very large even when the 2D order is relatively strong. For example, for a system in which the order parameter is 70% of the largest possible value, $L_y = 8$ is required for ordering. Extrapolations of the VBS order parameter based on correlation functions (the square of the order parameter) for small $L \times L$ lattices can also be misleading. For a 20%-ordered system results for $L$ up to $\approx 20$ appear to extrapolate clearly to a vanishing order parameter, while for larger lattices the scaling behavior crosses over and extrapolates to a non-zero value (with exponentially small finite size corrections).

The VBS order parameter also exhibits interesting edge effects related the known emergent $U(1)$ symmetry close to a “deconfined” critical point, which, if not considered properly, can lead to wrong conclusions for the thermodynamic limit. The observed finite-size behavior for small $L \times L$ lattices and long cylinders is very similar to that predicted for a $Z_2$ spin liquid. The results therefore raise concerns about recent numerical work claiming $Z_2$ spin liquid ground states in 2D frustrated quantum spin systems, in particular, the Heisenberg model with nearest and next-nearest-neighbor couplings. Based on the results presented so far, a VBS state in this system cannot be ruled out.

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I. INTRODUCTION

A valence-bond solid (VBS) is a state of a quantum spin system in which there is no magnetic long-range order, but lattice symmetries (translational and some times rotational) are broken due to dimerization or, more generally, polymerization of the system into one with a larger unit cell than the underlying lattice. One can think of the spins within a unit cell of a VBS (or within different groups of spins in a large complex unit cell) as having an enhanced probability of forming a total spin singlet. In this paper, manifestations of VBS order in ground states of finite systems are investigated, using unbiased quantum Monte Carlo (QMC) simulations of $S = 1/2$ spins on the two-dimensional (2D) square lattice with interactions—Heisenberg exchange supplemented by certain multi-spin interactions—leading to columnar order in the thermodynamic limit. The approach to the infinite-size 2D limit is investigated for different boundary conditions. The models considered can be tuned from strong to weak VBS order (and also through a critical point), enabling bench-mark investigations of asymptotics and cross-over behaviors. In particular, consequences of near-criticality of the VBS order on the finite-size behavior can be examined in detail. The stability of VBS order on long cylinders ($L_x \times L_y$ lattices with $L_x \gg L_y$) is also addressed. This geometry is often used in density matrix renormalization (DMRG) studies with recent intriguing results pointing to the absence of VBS order and the existence of spin liquids in frustrated models whose ground states have been debated for a long time.

In the following introductory sections, several background facts motivating further studies of VBS order are discussed and some of the known properties of VBS states are briefly reviewed. The purposes of the studies reported here will then be detailed, followed by an outline of rest of the paper.

A. VBS states and frustrated interactions

VBS states have been known for a long time to exist in 1D frustrated quantum spin chains. In particular, in the $S = 1/2$ Heisenberg chain with nearest- and next-nearest-neighbor couplings $J_1$ and $J_2$, the ground state at coupling ratio $g = J_2/J_1 = 1/2$ is exactly a product of singlets formed on alternating nearest-neighbor bonds (a pattern which can be realized in two different ways; hence the ground state is two-fold degenerate). Away from this special, exactly solvable point, there are fluctuations modifying the simple product state. Numerical exact diagonalization studies have shown that long-range dimerization survives down to $g_c \approx 0.241$. For $g < g_c$, the ground state exhibits critical spin and VBS correlations (like the standard Heisenberg chain with $J_2 = 0$). Away from this special, exactly solvable point, there are fluctuations modifying the simple product state. Numerical exact diagonalization studies have shown that long-range dimerization survives down to $g_c \approx 0.241$. For $g < g_c$, the ground state exhibits critical spin and VBS correlations (like the standard Heisenberg chain with $J_2 = 0$).
At higher $g$, the simple dimer VBS order persists at least up to $g \approx 0.6$, above which more complicated VBS or spiral spin states likely form. The frustrated 2D square-lattice $J_1$-$J_2$ Heisenberg model (with nearest-neighbor couplings $J_1$ and the $J_2$ interactions connecting spins across the diagonals of each four-spin plaquette) also has a non-magnetic ground state in some window of coupling ratios $0.4 \lesssim g \lesssim 0.6$ (outside of which the ground state is Néel antiferromagnetic for smaller $g$ and exhibits stripe antiferromagnetic order for larger $g$). However, in this case it has been difficult to determine the exact nature of the ground state. Many studies over the past two decades have suggested a VBS, with either columnar or plaquette (four-spin unit cell) order but spin liquid ground states (which have no broken symmetries but may have topological order) have also been proposed. Very recently, results of DMRG calculations on cylindrical semi-periodic lattices (with open edges in one direction—see Fig. 1) were used to argue more specifically that the ground state of the system for $0.41 \leq g \leq 0.62$ is a $Z_2$ spin liquid. A concurrent calculation based on tensor-product states also claimed the absence of VBS order.

A story similar to that of the $J_1$-$J_2$ Heisenberg model has played out in recent years in the case of the $S = 1/2$ Heisenberg model with only nearest-neighbor interactions on the geometrically frustrated kagome lattice. Many calculations initially suggested a VBS ground state (in this case with a complex 12- or 36-site unit cell) but the most recent DMRG studies support a $Z_2$ spin liquid scenario (as also predicted in early analytical work). Here, as well, cylindrical lattices played a crucial role in obtaining the numerical data.

**B. Deconfined quantum-critical points and VBSs with emergent U(1) symmetry**

When the Néel order of a 2D antiferromagnet such as the $S = 1/2$ Heisenberg model is destroyed in a continuous quantum phase transition, one scenario is that the putative spin-liquid state is immediately unstable to the formation of a VBS. This has been argued to lead to a "deconfined" quantum-critical point separating the Néel and VBS states. The phase transition is associated with deconfinement of spinons. Being generically continuous, due to subtle quantum interference effects, this type of transition violates the classical "Landau rule", according to which a transition between two ordered states breaking unrelated symmetries should be generically first-order.

In the low-energy field-theory argued to describe the deconfined quantum-critical point (the 2+1 dimensional non-compact CP$^1$ theory) the VBS fluctuations correspond to a U(1) gauge field to which spinons are coupled. There is a dangerously irrelevant operator (a quadrupled monopole operator) which reduces the U(1) symmetry to a four-fold ($Z_4$) symmetry inside the ordered VBS state (in which the spinons become confined). On the square lattice, this corresponds to the four degenerate columnar VBS patterns. Close to the critical point, the $Z_4$ symmetry only becomes apparent beyond a length-scale $\Lambda$, which is larger than the standard correlation length $\xi$ associated with the magnitude of the order parameter. At distances below $\Lambda$ there are angular fluctuations of the VBS order parameter ($D_x$, $D_y$), which in a system with $x$ order, $|D_x| > 0, D_y = 0$, induces $D_y$ order on length scales up to $\Lambda$, with this length diverging as $\Lambda \sim \xi^{1+a}$ with $a > 0$. At distances much below $\Lambda$, the angle of the VBS order parameter fluctuates in an essentially U(1) isotropic manner.

The deconfinement scenario appears to be realized in a class of "$J$-$Q$" models in which the Heisenberg exchange $J$ is supplemented by certain multi-spin interactions—products of two or more two-spin singlet projectors acting on different spin pairs. These interactions lead to the formation of local correlated singlets, thereby reducing, and eventually destroying, the Néel order. Results of QMC calculations (which are not affected by sign problems in this case) are consistent with a single critical point separating the Néel state and a VBS. While some works suggested that the transition is weakly first-order, the most recent studies point to a continuous transition with anomalously large scaling corrections. Moreover, emergent U(1) symmetry has been explicitly observed in the VBS order parameter distribution. By studying the U(1) - Z$_4$ cross-over, the exponent $a$ was estimated in Ref. to be $a = 0.20 \pm 0.05$.

**C. Stability of the spin liquid**

For the frustrated spin systems discussed above in Sec. I A deconfined quantum-criticality, i.e., a gapless spin liquid existing only at a singular point, is also an alternative to the transition out of the Néel state into an extended spin liquid phase. At the heart of this issue is the question of the stability of the spin liquid state. The deconfined quantum-criticality scenario implies that some spin liquids are generically unstable, at least under some commonly satisfied conditions, but stable spin liquids can also exist.
Recently Cano and Fendley succeeded in constructing a long-sought local (but complicated) Hamiltonian\(^2\) that is the parent Hamiltonian of the prototypical resonating valence bond (RVB) spin liquid, i.e., the equal superposition of all nearest-neighbor valence bond configurations (with the Marshall sign rule built in)\(^3\). This state, however, is a U(1) spin liquid with exponentially decaying spin correlations but critical VBS correlations\(^4,5\), and not the kind of fully gapped Z\(_2\) spin liquid proposed in the context of the frustrated models discussed above [but a U(1) spin liquid is also a possible ground state candidate of this model\(^6\)]. As a consequence of its close relationship with the critical Rokhasr-Kivelson dimer model\(^7,8\), one would expect this state to be generically unstable to perturbations of the Cano-Fendley Hamiltonian, leading to the formation of a VBS. Viewed from the perspective of a class of quantum states, the introduction of longer bonds either maintains the critical VBS\(^9\) or leads to a Z\(_2\) spin liquid\(^10,11\) but the Hamiltonian for these extended RVB states is not known.

Stable Z\(_2\) spin liquids are known with Klein Hamiltonians on particular decorated lattices\(^12\) but the degree of stability of these states when moving away from the limit of high decoration is not known. The Kitaev honeycomb-lattice model\(^13\) which has a Z\(_2\) liquid state, can also be related to a model of SU(2) interacting spins on a decorated honeycomb lattice\(^14\). However, there is still no rigorously known example of a Z\(_2\) spin liquid ground state of a local SU(2) invariant Hamiltonian on one of the simple standard 2D lattices (square, triangular, honeycomb, kagome, etc.). This lack of a prototypical system underlies the quest to find Z\(_2\) liquids in numerical studies of frustrated quantum spin Hamiltonians\(^15\). Z\(_2\) spin liquid states have already been confirmed in QMC studies of frustrated quantum XY models\(^16\).

D. Detection of spin liquids and VBS order

It is highly non-trivial to unambiguously confirm 2D spin liquid states based on numerical calculations on relatively small lattices. The main difficulty here is to exclude weak VBS order (while the absence of magnetic order is easier to confirm, e.g., by demonstrating a non-zero spin gap). There is therefore much interest in finding positive signals for various spin liquid phases, e.g., using unique finite-size scaling properties of the entanglement entropy\(^17,18\). Other signals related to the topological aspects of spin liquids have also been proposed\(^19,20\). However, regardless of what properties are investigated, great care has to be taken in view of the small lattices accessible for systems with frustrated interactions. Due to sign problems, unbiased QMC studies of the ground states of these systems are essentially impossible\(^21\), (although some progress has been made here recently at elevated temperatures\(^22\)). Variational QMC methods can be used\(^23\) but are not reliable, because very different states can have almost the same energy. Exact diagonalization studies can reach \(\approx 42\) spins\(^24\),\(^25\) while DMRG calculations now can reach hundreds of spins\(^2\). Tensor-product state methods (which can be regarded as generalizations of the matrix-product based\(^26\) DMRG scheme) can reach much larger sizes, but are complicated by the fact that extrapolations also have to be carried out in the bond dimension of the tensors\(^27,28,29\). In DMRG calculations there is a similar issue with regards to the maximum number of states that can be kept, which is what limits the accessible system sizes (since that number of states in this case has to grow exponentially with the system size).

E. Lattice shapes and boundaries

As already mentioned, in DMRG studies it has become popular to use lattices in the form of cylinders with semi-periodic boundary conditions (with periodic boundaries along the long direction and open short edges), as illustrated in Fig. 1. An aspect ratio \(L_x/L_y > 1\) improves the convergence with the number of states kept, as compared to a fully periodic lattice with equal length in both directions (for a given total number of lattice sites)\(^2\). The better convergence with samples of this shape can be traced to the inherently 1D nature of the DMRG procedures and how the generated states can incorporate entanglement\(^28\). It has also been argued that cylindrical \(L_x/L_y > 1\) samples, some times in combination with modifications of the boundaries (e.g., using field terms breaking some symmetry), have other favorable effects, as well on the convergence of various order parameters as a function of the system size\(^23\).

In QMC studies of sign-problem free models, periodic \(L \times L\) lattices are normally used. In cases where the couplings are spatially anisotropic, it has proved helpful to use \(L_x \times L_y\) lattices with \(L_x \neq L_y\), while in other cases no particular advantages of such rectangular lattices were noted\(^29\). Open boundaries have been considered in QMC work primarily in cases where the perturbing effects of the edges are the actual targets of investigation\(^30,31\). In a previous QMC study of a VBS state it was also noted that open boundaries can be used to break the four-fold symmetry of the 2D VBS completely and stabilize a unique VBS pattern, as an alternative of studying VBS correlation functions in periodic lattices with no explicitly broken symmetries\(^32\).

F. Purpose of the paper

The main purpose of the present paper is to systematically investigate the role of the lattice shape and boundary conditions on the finite-size scaling properties of the VBS order parameter. VBS states have in the past few years been conclusively demonstrated in several 2D \(J-Q\) models\(^33,34,35,36,37\) and also in 1D chains (where the same kind of dimerization transition takes place as in
the frustrated $J_1$-$J_2$ chain and 3D systems. Different types of VBS patterns can be realized, depending on the arrangements of the singlet projectors on the lattice. These models have been studied with large-scale QMC simulations, mainly for the purpose of investigating the nature of the Néel–VBS transition. Here the main focus will instead be on the VBS state itself (including its cross-over behavior close to criticality), using the $J$-$Q$ models to obtain generic benchmarks for finite-size scaling of this kind of order parameter. An efficient approximation-free ground state projector QMC method was used to obtain results for both strongly and weakly VBS ordered systems on square lattices with different shapes and boundaries.

In order to make contact with the currently favored manner of applying the DMRG method to cylindrical systems with open edges in one direction will be studied extensively. The convention adopted here is that the edges parallel to the $y$-axis are open, and periodic boundary conditions are applied in the other direction. Such an $L_x \times L_y$ lattice is illustrated in Fig. [1] In some cases the open edges will be modified to favor a certain VBS pattern, which is often also done in DMRG studies. Fully periodic lattices will also be considered. Two aspect ratios, $L_x/L_y = 1,2$, will be considered for both the semi- and fully periodic systems. The limit $L_x \to \infty$ will also be taken for small $L_y$.

In addition to suggesting optimal approaches for extracting the VBS order in the 2D thermodynamic limit, the results presented here will also show that the issue of excluding VBS order in a system with an unknown type of non-magnetic ground state may be more difficult than what has been anticipated so far. In particular, the geometry of long cylinders can give misleading results. Not only can calculations on such systems completely miss 2D VBS order (because the system is disordered with a short correlation length on the cylinders), but also the claimed positive signals of a 2D $\mathbb{Z}_2$ spin liquid cannot be trusted when used with cylinders of practically accessible widths (because they are essentially 1D spin liquids although the state orders in the 2D limit). The emergent $U(1)$ symmetry of the VBS state leads to interesting boundary effects, which are also studied here.

G. Outline of the paper

In Sec. II the $J$-$Q$ models are specified in detail, the correlation functions of interest are defined, the projector QMC method is briefly outlined, and its convergence properties are discussed and illustrated with an example. Extrapolations of the infinite-size value of the order parameter is discussed in Sec. III Results for the $J$-$Q_3$ model at $J = 0$ (the pure $Q_3$ model), which has very robust columnar VBS order, is discussed first, in order to show how the different ways of extrapolating the order parameter to the thermodynamic limit agree well with each other. Results for three different lattice types are compared; periodic $L \times L$ and $2L \times L$ systems as well as semi-periodic cylindrical $2L \times L$ systems. The much weaker VBS ordering in the $Q_2$ and $J$-$Q_2$ models is discussed next, using the same lattices as above. Here several subtle issues are pointed out that affect extrapolations to infinite size when the order is not strong, and, therefore, the length-scales $\xi$ and $\Lambda$ are large. The quantum-critical scaling form of the VBS order parameter is also discussed, as a nearby critical point also influences the finite-size behavior in systems off criticality. The vector aspects of the columnar VBS order parameter $(D_x, D_y)$ and the effects of its emergent $U(1)$ symmetry are studied in detail in Sec. IV The evolution of the $x$- and $y$-components of the order parameter as a function of the distance from an open edge is studied, with and without symmetry-breaking modifications of the edge. In Sec. V the destruction of VBS order on cylinders is studied in the limit $L_x \to \infty$ and $L_y$ fixed. The most important results are summarized and their implications are discussed in Sec. VI Here detailed comparisons with the recent DMRG results for the $J_1$-$J_2$ Heisenberg model are also made. Detection of the $U(1)$–$\mathbb{Z}_4$ symmetry of the VBS order parameter based on probability distributions $P(D_x, D_y)$ generated in QMC calculations is discussed in Appendix A.

II. MODELS AND METHODS

A. J-Q models

A generic $J$-$Q$ model is defined using products of singlet projectors $C(i,j)$ on two sites,

$$C(i,j) = \frac{1}{4} - S_i \cdot S_j. \quad (1)$$

The standard Heisenberg model is just a sum of such singlet projectors over the interacting bonds $(i,j)$ (here nearest-neighbor sites on the square lattice),

$$H_J = -J \sum_{\langle i,j \rangle} C(i,j), \quad (2)$$

where the minus sign corresponds to antiferromagnetic interactions. A $Q_n$ term consists of products of two or more $(n)$ singlet projectors acting on different bonds;

$$H_{Q_n} = -Q_n \sum_{a} \prod_{b=1}^{n} C(i[a,b], j[a,b]). \quad (3)$$

Here $a$ is a label corresponding to the lattice units within which the singlet projectors are arranged and $b$ labels the bonds (spin pairs) on which the singlet projectors within these units act; $i[a,b]$ and $j[a,b]$ above refer to the two sites connected by bond $b$ in unit $a$. In the simplest kind of $Q_2$ term on the square lattice, $a$ denotes $2 \times 2$ plaquettes, with the two projectors within these plaquettes connecting spins either horizontally or vertically (i.e., for
The expectation value is written as

\[
\langle \mathcal{O} \rangle = \sum_{\mathbf{P}} \langle \mathcal{O} \mid \mathbf{P} \rangle P(\mathbf{P})
\]

where \( \langle \mathcal{O} \mid \mathbf{P} \rangle \) is the string \( \mathbf{P} \) indexed by \( \mathbf{O} \).

When \( \langle \mathcal{O} \rangle \) does not break any of the symmetries of the lattice. The sum over projectors is such that the Hamiltonian does not have QMC sign problems and can be studied with any efficient QMC loop algorithms. Here the ground state is the pure valence bond basis in the singlet sector. The convergence of \( \langle \mathcal{O} \rangle \) to the true ground state expectation value \( \langle \mathcal{O} \rangle_0 \) is then dictated by the gap to the second singlet.

FIG. 2: (Color online) \( Q_2 \) and \( Q_3 \) terms on the square lattice. The bars of length one lattice constant indicate the locations of singlet projectors \( C(i,j) \) on site pairs \( i,j \). The Hamiltonian contains all unique translations of these operators.

When a \( Q \) term is present are straightforward and have been discussed briefly in Ref. 10: First all the operators in the \( J \) and \( Q \) terms are split into their diagonal and off-diagonal components in the basis of spin states \( |S_i^z, \ldots, S_N^z\rangle \) used. The diagonal operators can be moved around on the lattice as long as each operator is compatible with the spin state on which it acts (with only operators on anti-parallel spins allowed). The full set of operators is sampled by changing the types of some operators from diagonal to off-diagonal, or vice versa, on the same lattice unit \( a \), using an efficient loop algorithm.

The ground state of a bipartite \( J-Q \) model (i.e., with each singlet projector connecting two spins on different sublattices) being guaranteed to be singlet, it is particularly convenient to use a trial state expressed in the valence bond basis in the singlet sector. The convergence of \( \langle \mathcal{O} \rangle \) to the true ground state expectation value \( \langle \mathcal{O} \rangle_0 \) is then dictated by the gap to the second singlet. For a periodic lattice (or a semi-periodic cylinder), a transitional-invariant trial state also filters out excited states with non-zero momentum from the outset. Translational invariance in the applicable lattice direction(s) is easily ensured by using an amplitude-product state for \( |\Psi_0\rangle \), i.e., a superposition written in terms of bipartite valence bond states \( |v\rangle \),

\[
|\Psi_0\rangle = \sum_v c_v |v\rangle.
\]

Here the sum includes all tilings of the \( N \)-site lattice into \( N/2 \) bipartite two-spin singlets, i.e.,

\[
|v\rangle = \prod_{i=1}^{N/2} (|i, j_i\rangle - |j_i, i\rangle) / \sqrt{2}
\]

where \( (i, j) = (|l, j_i\rangle - |j_i, l\rangle) / \sqrt{2} \) with \( i \) and \( j \) sites on sublattice \( A \) and \( B \), respectively, and the weight \( c_v \) of a given tiling \( v \) into singlets depends only on the “shapes” \( l = (l_x, l_y) \) of the bonds in \( |v\rangle \);

\[
c_v = \prod_l h(l)^{n_l},
\]

where \( n_l \) is the number of bonds of shape \( l \).

Amplitude-product states are very easy to sample in the course of the projection according to \( D \), as also described in Ref. 31. The detailed form of the amplitude \( h(l) \) is not crucial when the state is used as a trial state. Variationally optimized amplitudes lead to faster convergence with the power \( m \), but even without optimizing the convergence properties are good. In the work reported here, amplitudes decaying with the bond length \( l \) as \( l^{-3} \) were used (in which case the trial state itself has Néel order, but this is very quickly destroyed by the projection procedure in a VBS state).

B. Projector QMC

\( J-Q \) models with minus signs as in Eqs. (2) and (3) do not have QMC sign problems and can be studied with very efficient QMC loop algorithms. Here the ground state projector method developed in Ref. 81 is used. It is based on applying a high power of the Hamiltonian to a “trial” state \( |\Psi_0\rangle \),

\[
|\Psi_m\rangle = (-H)^m |\Psi_0\rangle,
\]

where \( (-H)^m \) is written as a sum over all possible strings of the individual \( J \) and \( Q \) terms in (2) and (3). Denoting such a string of singlet projectors by \( P_m(i) \), with \( i \) formally indexing the different strings, an operator expectation value is written as

\[
\langle A \rangle_m = \frac{\sum_{ij} \langle \Psi_0 | P^T_m(j) A P_m(i) | \Psi_0 \rangle}{\sum_{ij} \langle \Psi_0 | P^T_m(j) P_m(i) | \Psi_0 \rangle},
\]

where \( P^T_m(j) \) is the string \( P_m(j) \) in reverse order.

The QMC method implements importance sampling of the operator strings \( P^T_m(j) P_m(i) \), which is done in two steps, as described in detail in Ref. 81 in the case of the Heisenberg model (and the modifications of the scheme.
C. Correlation functions

In order to characterize the ground state, the spin ($s$) and dimer ($d$) correlation functions are computed. These are defined in the standard way as

$$C_s(r_{ij}) = \langle S(r_i) \cdot S(r_j) \rangle,$$  \hspace{1cm} (9)

$$C_d(r_{ij}) = \langle B_\alpha(r_i) B_\alpha(r_j) \rangle,$$  \hspace{1cm} (10)

where $r_{ij} = r_i - r_j$ is the spatial separation of the operators and $B_\alpha$, $\alpha = \hat{x}, \hat{y}$, is the dimer operator on nearest-neighbor bonds oriented in the $\alpha$ direction, e.g., for $\alpha = \hat{x}$

$$B_\hat{x}(r) = S(r) \cdot S(r + \hat{x}).$$  \hspace{1cm} (11)

One can also define cross-correlations $\langle B_\alpha(r_i) B_\beta(r_j) \rangle$ but they will not be needed here. The correlation functions can be easily computed using loop estimators based on the transition graphs generated when the sampled valence bond states in the ket and bra states of Eq. (15) are propagated by the string of singlet projectors. The estimators are discussed in detail in Refs. 77 and 85.

Columnar and plaquette VBS states can both be detected by the columnar VBS order parameter, which can be defined by the operators

$$D_x = \frac{1}{N} \sum_{x,y} B_x(x,y)(-1)^x,$$  \hspace{1cm} (12)

$$D_y = \frac{1}{N} \sum_{x,y} B_y(x,y)(-1)^y.$$  \hspace{1cm} (13)

In a columnar state with the lattice rotational symmetry completely broken, either $D_x$ or $D_y$ has a non-zero expectation value, while in a plaquette state they are both non-zero and equal. The $J$-$Q$ models studied here host only columnar VBS states. However, as we will be discussed below, in a columnar state on a finite lattice one can have both non-zero $\langle D_x \rangle$ and $\langle D_y \rangle$, due to boundary and shape effects.

In periodic and semi-periodic systems where the degeneracy of the possible VBS patterns is not broken, one can only detect the VBS with the corresponding correlation functions, e.g., the squares of the order parameters defined above. In particular, it is useful to consider the total squared order parameter,

$$D^2 = D_x^2 + D_y^2.$$  \hspace{1cm} (14)

The magnitude of the order parameter in a corresponding symmetry-broken state is $D = (D^2)^{1/2}$ (which can be taken as a definition of the value $D$ of the order parameter). In non-square samples it is also illuminating to investigate the components $\langle D_x^2 \rangle$ and $\langle D_y^2 \rangle$ individually, to see how the lattice shape (and boundaries) affect the symmetry breaking. As will be demonstrated in the following sections, this issue is, in fact, of key importance for interpreting numerical results for non-square samples.

In the cylindrical semi-periodic systems it is useful to define the order parameter in such a way that the perturbing effects of the open edges are partially eliminated. As in Ref. 6, for such systems with $L_x > L_y$ the summations in (12) and (13) will normally be taken over only the central sites within a square of size $L_y \times L_y$.

In cases when the lattice coordinates $(x, y)$ are needed explicitly in the further discussion of correlation functions in the later sections, the numbering convention will be $x \in \{0, \ldots, L_x - 1\}$ and $y \in \{0, \ldots, L_y - 1\}$.

D. Convergence tests

To examine the convergence properties of the projector method, the state (1) after $m$ operations with $H$ can be written in terms of eigenstates $|n\rangle$ of $H$ as

$$|\psi_m\rangle = \sum_n c_n |E_n^m |n\rangle,$$  \hspace{1cm} (15)

where $c_n$ are the expansion coefficients of the trial state in the energy basis. Assuming that the ground state energy $E_0$ is the largest in magnitude, $|E_0| \geq |E_n|, \ \forall \ n > 0$, which is the case for sure with a Hamiltonian expressed using the singlet projectors (1) and the signs as in (2) and (3), an expectation value of an operator $A$ not commuting with the Hamiltonian can be expanded as

$$\langle A \rangle_m = \langle 0 | A | 0 \rangle + 2 \langle 1 | A | 0 \rangle \frac{c_1}{c_0} \left( \frac{E_1}{E_0} \right)^m + \ldots.$$  \hspace{1cm} (16)

Here $|1\rangle$ is the first excited state in the symmetry sector considered, which with an amplitude product state obeying all applicable lattice symmetries is a singlet that is fully symmetric with respect to all the symmetry operations (translations, reflections, and rotations of the lattice). With the gap $\Delta = E_1 - E_0$ and a large projection-power $m$, Eq. (16) can be written as

$$\langle A \rangle_m = \langle 0 | A | 0 \rangle + c \exp \left( - \frac{m}{N} \frac{\Delta}{|e_0|} \right),$$  \hspace{1cm} (17)

where $e_0$ is the ground state energy per site, $e_0 = E_0/N$, and $c$ is a constant. In order to achieve good convergence, one should therefore use a size-normalized projection power $m/N \gg 1/\Delta$.

The gapped VBS state being of primary interest here, $\Delta/e_0$ approaches a non-zero constant as the system size increases. One may then expect good convergence properties with an essentially size independent $m/N$. However, for system sizes accessible in practice, the gap still typically decreases significantly with the system size. In addition, the density of states above the gap increases as well. As a consequence, $m/N$ has to be increased with the system size to ensure good convergence. Since the number of operations required for one full sweep of Monte Carlo updates of a configuration in the projector method is of order $m^2$, the computation time in practice grows faster than $N$. 

All results presented here were tested for convergence by carrying out several calculations with different projection powers $m/N \propto L$ (with $L = \max[L_x,L_y]$ for non-square lattices) and making sure that there is no remaining detectable dependence on $m$. An example of a detailed convergence test is shown in Fig. 3. Typically, $m/N = L/2$ was sufficient to ensure good convergence. In principle the singlet-singlet gap can be extracted by fitting the exponential form (17) to data such as those in Fig. 3 (as shown in the inset), but such gaps will not be studied here.

III. EXTRAPOLATION OF VBS ORDER

Previous ground-state and finite-temperature QMC studies have confirmed that both the $J$-$Q_2$ and $J$-$Q_3$ models, with the singlet projectors arranged as in Fig. 2, have VBS-ordered ground state for large $Q_n/J^{1.4,18,21}$. The maximal order parameter obtains for $J = 0$ (pure $Q_2$ models) and, naturally, the order is more robust in the $Q_3$ model. The previous studies were mainly concerned with the critical and near-critical aspects of the Néel and VBS order parameters—the critical exponents as well as the emergent $U(1)$ symmetry seen in the VBS order parameter $(D_x,D_y)$.

In this section some important aspects of the VBS order parameter will be discussed first, in particular the expected consequences of its emergent $U(1)$ symmetry. Then, turning to numerical results, the magnitude of the VBS order parameter of the pure $Q_3$ model will be extracted first, to illustrate the convergence as a function of the lattice size for several cases of lattice shapes and boundary conditions. The $J$-$Q_2$ model, including the pure $Q_2$ case, is then considered in order to investigate potential problems arising when the VBS order is weaker. The quantum-critical scaling will also be discussed briefly, as it is directly related to the extrapolation problems when the VBS can be considered near-critical.

A. Nature of the VBS order parameter

Note first that the maximal columnar VBS order parameter is obtained for the state with no fluctuations in the valence bond basis—the state with nearest-neighbor singlets on all bonds of every second column. If the singlets are oriented in the $x$ direction, then the order parameter components defined in (12) and (13) have the expectation values $\langle D_x \rangle = 3/8$ (up to an arbitrary sign) and $\langle D_y \rangle = 0$. If the symmetry is not broken and the ground state is an equal superposition of the four degenerate valence-bond states with horizontal and vertical bonds, then the expectation value of the squared VBS order parameter $\langle D^2 \rangle = 9/64$ in the limit of an infinitely large system. For finite systems there are corrections to this value, however, which are related to the non-orthogonality and over-completeness of valence bond states $^{20,35}$.

The emergent $U(1)$ symmetry property of the VBS order parameter $\langle D^2 \rangle$ and its related length-scale $\Lambda$ will be of importance in order to understand many of the results to be discussed here and in the later sections. For $L \ll \Lambda$, the order parameter $(D_x,D_y)$ on an $L \times L$ lattice behaves essentially as an isotropic 2D vector, while for $L \gg \Lambda$ the order parameter locks to one of the four angles $\pi/2$. This is further discussed in Appendix A. Here, for $L_x \neq L_y$ lattices, with or without open edges, the $U(1)$-$Z_4$ cross-over will manifest itself also in how (on what length scale) the $90^\circ$ rotational symmetry of the VBS order parameter is broken on a lattice which does not have this symmetry.

It should be noted that symmetry cross-overs such as the $U(1)$-$Z_4$ case discussed here also occur in many classical systems with dangerously irrelevant perturbations (i.e., ones that do not change the universality class of a phase transition but reduce the degeneracy of the ordered state), e.g., the 3D XY-model with a $q$-fold symmetry-breaking field of the form $\cos(q\theta_i)$ (with $q \geq 4$). There are several numerical studies of the scaling dimension of such a dangerously irrelevant perturbation and the nature of the cross-over and its length-scale $\Lambda$. $^{20,38,39}$

B. Strong VBS order in the pure $Q_3$ model

Fig. 4 shows the size dependence of $\langle D^2 \rangle$ of the $Q_3$ model computed on periodic $L \times L$ and $2L \times L$ lattices. For the latter systems the individual expectation values $\langle D_x \rangle^2$ and $\langle D_y \rangle^2$ are also shown (while these are of course both equal to $\langle D^2 \rangle/2$ for the $L \times L$ lattices). Here convergence of $\langle D^2 \rangle$ to a non-zero value when $L \rightarrow \infty$ is apparent for both types of lattices. It is interesting to note that both the $x$ and $y$ components are nonzero on the $2L \times L$ lattices for small $L$, but for larger systems
the symmetry is completely broken, eventually leading
to \( \langle D_x^2 \rangle \rightarrow 0, \langle D_y^2 \rangle \rightarrow \langle D^2 \rangle \). Thus, on the non-square
periodic lattices the columnar state with the bonds or-
eted parallel to the shorter lattice direction (here \( L_y \)) is
ergetically favored. This remains true also for larger
aspect ratios \( L_x/L_y \).

The cross-over from partially broken to fully broken \( x-y \) rotation symmetry, which in Fig. 4 takes place for the
\( 2L \times L \) systems for \( L \approx 20 \), should be related to the emer-
gent \( U(1) \) symmetry of the VBS order parameter. As discussed in Appendix A for the \( Q_3 \) model no per-
fect \( U(1) \) symmetry can be detected on periodic \( L \times L \) lattices (since the length-scale \( \Lambda \) is very short), but for a
wide range of sizes the system is in a cross-over regime be-
tween \( U(1) \) and \( Z_3 \) symmetry. The range of \( L \) over which
the cross-over to a purely \( y \)-ordered VBS takes place in
Fig. 4 is roughly where all traces of \( U(1) \) symmetry van-
ish on the \( L \times L \) lattices (as discussed in Appendix A).

Turning now to the quantitative behavior of the to-
tal order parameter for the largest systems in Fig. 4 as
expected the order parameters for both lattice types ex-
trapolate to the same value in the thermodynamic limit.
Fits of the data for the largest systems to second-order
polynomials are shown. Note, however, that this form is
strictly not correct. For a discrete broken symmetry one
would expect the asymptotic finite-size corrections to be
exponentially decreasing with increasing system size. It
is not easy to reach sufficiently large systems to observe
this behavior, however. The second-order fits look rea-
sonably good on the scale of the plot, but in fact they are
not of high quality statistically when 6-8 data points are
included. Including higher powers helps somewhat, but
this can lead to fitted forms that do not behave monoton-
ically as \( 1/L \rightarrow 0 \). Such problems with the polynomial
fits reflect a cross-over to the eventual exponentially rapid
convergence. Using second-order fits for the largest few
system sizes still should result in a reasonably accurate
extrapolated order parameter. Normally such an extrap-
olation should give a lower bound on the actual value, but
this cannot be guaranteed in the presence of statistical
errors. In the case considered here, the results for \( L \times L \)
and \( 2L \times L \) extrapolate to 0.0691 and 0.0684, respectively,
with the fits shown in Fig. 4. Because of the issues with the,
strictly speaking, wrong form of the fitting func-
tion, it is not meaningful to compute error bars on these
numbers—the purely statistical errors are smaller than
the variations among fits with different polynomials and
number of data points included. For the purposes of the
investigations in this paper, the issue of statistical errors
is only of minor importance, however (while the system-
atical errors due to a wrong fitting form are important).

Data for cylindrical \( 2L \times L \) systems are shown Fig. 5. Here the order parameters are computed on the central
\( L \times L \) square. In sharp contrast to the fully periodic
\( 2L \times L \) systems, here it is the \( x \)-component of the order pa-
rameter that survives in the thermodynamic limit. Thus,
the open edges along the \( y \) direction favor the bonds or-
dering perpendicularly to them, and this effect wins over
the competing effect, demonstrated in Fig. 4 of the as-
pect ratio \( L_x/L_y > 1 \) favoring bonds ordering in the \( x \)
direction. Quadratic fits to \( \langle D_x^2 \rangle \) and \( \langle D_y^2 \rangle \) for a few of
the largest system sizes extrapolate to 0.0685 and 0.0694,
respectively, in good agreement with the results for the periodic systems.

As a consequence of the open boundaries inducing an
\( x \)-oriented VBS, the ordering pattern in this case is non-
degenerate. Therefore, the unsquared order parameter
\( \langle D_x \rangle \) is non-zero and should, in the thermodynamic limit, take a value agreeing with the squared order parameters.
ordered along the edges but remains large also in the interior of the system. The dimer order is clearly the strongest at the location of the nearest-neighbor spin correlator indeed oscillates considerably as a function of the location along the axis. This quantity at the central column is shown as a function of the inverse system size in the main plot of Fig. 6. Here an asymptotic exponentially fast convergence can be seen clearly, which is illustrated with a fit to the data, while the dashed black curve shows a quadratic fit to only the \( L \geq 20 \) data. The inset shows the behavior for the largest systems on a more detailed scale.

![Graph](image)

**FIG. 6:** (Color online) Local columnar \( x \) order parameter \( \langle D_x \rangle \) of the \( Q_3 \) model computed at the center of a \( 2L \times L \) cylinder. The smooth curve is of the exponential form and extrapolates to 0.264. The inset shows the location dependent bond correlation function \( \langle B_x(x) \rangle \) for a \( 32 \times 16 \) system.

extracted above: \( \langle D_x \rangle \rightarrow \langle D^2 \rangle^{1/2} \). The expectation value of the nearest-neighbor spin correlator indeed oscillates considerably as a function of the location along the \( x \) direction, as shown in the inset of Fig. 6 for the \( 32 \times 16 \) cylinder. The dimer order is clearly the strongest at the edges but remains large also in the interior of the system.

A local VBS order parameter for a system with bonds ordered along the \( x \) axis can be defined as

\[
D_x(x) = \langle B_x(x, y) \rangle - \frac{1}{2} \langle B_x(x-1, y) + B_x(x+1, y) \rangle, \tag{18}
\]

which is independent of \( y \) on the semi-periodic cylindrical lattices (and can be averaged over \( y \) in the QMC calculations). This quantity at the central column is shown as a function of the inverse system size in the main plot of Fig. 6. Here an asymptotic exponentially fast convergence can be seen clearly, which is illustrated with a fit to the form. This fit is of good statistical quality and extrapolates to 0.264, in good agreement with the values for \( \langle D^2 \rangle^{1/2} \) obtained above. The magnitude of the order parameter of the \( Q_3 \) model is, thus, 70% of the largest possible value (3/8) for a columnar VBS.

**C. Reduced order in the \( Q_2 \) and \( J-Q_2 \) models**

In the pure \( Q_2 \) model, the VBS order is considerably weaker than in the \( Q_3 \) model. The first study of this model gave the order parameter \( D \approx 0.070 \), or about 20% of the maximal value, based on extrapolations of \( L \times L \) results for \( L \leq 32 \). While this order may still be regarded as quite strong, problems with extrapolating it correctly based on small to moderate lattice sizes already start to become apparent.

Fig. 7 shows results for periodic \( L \times L \) systems with \( 4 \leq L \leq 72 \). A 5th-order polynomial can be fitted very well to all these data and extrapolates to 0.0063, about 10% lower than the previous result. However, if only \( L \geq 20 \) data are used, a second-order polynomial is sufficient and the extrapolated value is significantly lower; \( \langle D_x^2 \rangle = 0.0058 \). This illustrates the fact that polynomial fits based on small systems are not very reliable, because of the eventual exponential convergence (which is not yet fully apparent for the system sizes accessible). The resulting relative uncertainties are much larger than in the strongly ordered \( Q_3 \) model. The extrapolated value depends significantly on what system sizes are included in the fit and the order of the polynomial used. For the system sizes studied here, a pure exponential form does not yet work.

An important aspect of the finite-size scaling behavior in the \( Q_2 \) model is that the data for small to moderate lattices do not even clearly point to an ordered ground state. Fig. 7 also shows a second-order fit to only the \( L \leq 12 \) data points. The fit is statistically sound, but extrapolates to a negative value. Without access to larger system sizes it is not possible, using fitting procedures like this in \( 1/L \), to determine whether the ground state of the infinite 2D lattice is ordered or disordered. At least \( L = 20 \) is needed with \( 1/L \) extrapolations to definitely conclude that the ground state is ordered. It can be noted that an asymptotic \( \propto 1/L^2 \) behavior is expected if there is no long-range order, but this form should apply only for \( L \) much larger than the correlation length. Note that the correlation length itself is also not easy to extract from the correlation functions unless \( L \gg \xi \) (which is not the case here).

Fig. 7 shows results for periodic \( 2L \times L \) lattices. Using
polynomials to reliably extrapolate results to the infinite size limit is again difficult. An example using a 4th order polynomial with data for $L \geq 16$ is shown which extrapolates to $\langle D^2 \rangle = 0.0063$. Here it is again clear that the polynomial is not the correct form, because the fitted curve deviates significantly for the smaller systems not included in the fit.

The behavior of the individual $x$ and $y$ components in Fig. 8 appears to be qualitatively different from that observed in the $Q_3$ model (Fig. 4). In the more strongly ordered $Q_3$ model the $y$ component is always significantly larger than the $x$ component, and for large systems it completely dominates (the $x$ component vanishing). In the $Q_2$ model, the length-scale $\Lambda$ of the cross-over from U(1) to $\mathbb{Z}_4$ symmetry is much larger, and the dimer order parameter acts as an essentially isotropic vector even for the largest lattices considered here. A cross-over to a behavior where the $x$ component vanishes (as in the $Q_3$ model) should take place for larger system sizes, but, according to the analysis for $L \times L$ lattices in Appendix A, the cross-over length is beyond what can currently be studied with QMC calculations, with there being only weak signals of a columnar state. Since the two components are almost equal in magnitude in Fig. 8, it is clear that the fitted curve deviates significantly for the smaller systems not included in the fit. Thus, an example using a 4th order polynomial is not the correct form, because the fitted curve deviates significantly for the smaller systems not included in the fit.

It is interesting to note in Fig. 8 that the emergent $x$-$y$ symmetry is not manifested yet for the smallest systems. This reflects that the continuous angular nature of the VBS order parameter only appears upon coarse-graining and $L < 10$ is not sufficiently large for representing a continuous VBS angle. The two cross-over length-scales, into and out of an U(1) symmetric order parameter, have been investigated in detail in classical systems (clock models) exhibiting emergent U(1) symmetry.

As in the $Q_3$ model, on the open-edge cylinders with $L_x > L_y$ the favored VBS ordering pattern is that with the bonds primarily in the $x$-direction. Fig. 9 shows results for $2L \times L$ cylinders. Here the effect of the edges to strongly favor $x$ ordering overcomes the tendency to U(1) symmetry, and there is never any size range for which the $x$ and $y$ components are almost equal. Also here the behavior of both components for small lattices exhibit a naive extrapolation to a negative order parameter. For larger lattices ($D^2_x$) crosses over to a form extrapolating clearly to a non-zero value, while the $y$ component extrapolates to zero. A 4th-order polynomial fit to all the $x$-component data gives $\langle D^2_x \rangle = 0.0047$. This is significantly lower than the value quoted above for the examples of extrapolations of $L \times L$ data. However, the extrapolation is again sensitive to the lattice sizes included and the form of the fitting function used.

It is also useful to examine the long-distance VBS correlation function, which should contain less finite-size corrections to the infinite-size order parameter than the sums over all correlations. The squared order parameter $\langle D^2 \rangle$ contains significant non-asymptotic contributions from short distances. Using the real-space dimer correlation function defined in Eq. (10), the staggered part in the case of the $x$ component (and an analogous form for the $y$ component) can be extracted according to

$$C_{dx}^*(x, y) = \frac{1}{2}C_{dx}(x, y) - \frac{1}{4}[C_{dx}(x - 1, y) + C_{dx}(x + 1, y)],$$

where a factor $1/2$ has been included in order for $C_{dx}^*(x \to \infty, y) \to \langle D^2_x \rangle$, with $D_x$ defined in Eq. (10).
in the thermodynamic limit. Fig. 10 shows results for the longest distance on periodic $L \times L$ and $2L \times L$ lattices. For the $L \times L$ systems the sum of the $x$ and $y$ components is shown, along with a high-order polynomial fit that extrapolates to the infinite size order parameter $D^2 = 0.0061$. This extrapolation should be reasonably reliable, because the data for the largest systems flatten out clearly, reflecting the asymptotic exponential convergence (unlike the integrated quantity $\langle D^2 \rangle$ in Fig. 8 where no flattening-out is yet seen). For the $2L \times L$ system no reliable extrapolation is possible, because both components exhibit non-monotonic behavior. The sum of the $x$ and $y$ correlations for large $L$ is nevertheless very close to the $L \times L$ results.

It can also be noted in Fig. 10 that the individual components of the correlation function at long distance show somewhat less prominent $x$-$y$ symmetry than the integrated correlators in Fig. 8 although they are both still roughly equally large. Again, in the thermodynamic limit one of the components, likely the $x$ component, will have to turn down and vanish, as the $L_x > L_y$ geometry favors ordering in the $y$ direction.

In the previous section, it appeared that the most reliable way to extract the order parameter in the thermodynamic limit is to exploit the symmetry-breaking open edges, using $\langle D_x(x) \rangle$ defined in Eq. (18). Fig. 11 shows such results for open-edge cylinders of size $L \times L$ as well as $2L \times L$. Here the induced $x$ order appears to extrapolate to a value below the one obtained in Fig. 10 based on the long-distance correlation function—for the $2L \times L$ systems $\langle D_x(L - 1) \rangle$ is almost size independent for the largest systems, and one might hence conclude that it has converged. The square of this value is $\langle D_x^2 \rangle \approx 0.073^2 \approx 0.053$, which seems too low compared to the results in Fig. 10.

The reason for this apparent inconsistency should again be related to the emergent U(1) symmetry of the VBS order parameter: In addition to the $x$ component of the order parameter induced by the open edges, there still remains, for the accessible lattice sizes, a non-negligible $y$ component. This component is not locked-in by symmetry-breaking boundaries, however, but averages to zero if measured without first taking the square of its operator. The existence of a non-negligible fluctuating $y$ component nevertheless reduces the induced $\langle D_x \rangle$ from the full value, which should satisfy $D^2 = \langle D_x^2 \rangle + \langle D_y^2 \rangle$ for large systems. It is only when the system size exceeds the $U(1)$ length scale $\Lambda$ that one can expect the full order parameter to condense into the component $\langle D_x \rangle$, and this length scale cannot at present be reached for the $Q_2$ model. This shows again that the problem of extracting the VBS order parameter in the thermodynamic limit is a very delicate one.

The examples shown here demonstrate that, when the VBS order is relatively weak (the length scale $\Lambda$ is large), it is important to look at the full order parameter, including both the $x$ and $y$ components. The long-distance correlation function (Fig. 10) on $L \times L$ periodic lattices seems to be the fastest converging quantity, and it is in most cases best to use $L \times L$ lattices for extrapolations.

When turning on the Heisenberg exchange $J$, the VBS order of the $J$-$Q_2$ model is reduced and vanishes when $J/Q_2 \approx 0.045$. Here two cases are considered, $J/Q_2 = 0.03$ and 0.10, with the latter corresponding to a near-critical Néel state. Fig. 12 shows results for the total squared VBS order parameter and the staggered part of the dimer correlation function (averaged over the $x$ and $y$ directions. With $\langle D^2 \rangle$ graphed versus $1/L$ it is again difficult to extrapolate to infinite size based on small lattices. Here the lattices are nevertheless suf-
sufficiently large for it to be apparent that the system at 
$J/Q_2 = 0.03$ is VBS ordered, while for $J/Q_2 = 0.1$ the 
decay is much more rapid and consistent with no VBS or-
der. The corresponding long-distance correlations show 
these behaviors much more clearly, with the $J/Q_2 = 0.03$ 
data exhibiting the expected exponentially fast conver-
gence to a non-zero value for the largest sizes. Still, if 
data only for $L$ up to $\approx 10$ were available, it would not be 
possible to unambiguously confirm the presence of long-
range VBS order, even though the order parameter here 
is still above 10% of the maximum value.

Note that the long-distance correlation function de-
cays exponentially as a function of $1/L$ in a non-VBS 
state, i.e., much faster than the $1/L^2$ behavior of the total 
squared order parameter. It is therefore also much easier 
to confirm the absence of long-range order by studying 
the long-distance correlations.

D. Quantum-critical scaling

Ultimately, the difficulties in extrapolating the VBS or-
der parameter to infinite size based on small systems will 
in many cases be related to critical scaling in the proxim-
ity of a quantum-critical point (or “pseudo-critical” scal-
ing in cases where the transition out of the VBS state 
is weakly first-order). A small system exhibits quan-
tum criticality also slightly away from the critical point.
Hence, data for a series of lattices may appear to extrapo-
late to a disordered state, even though the infinitely large 
2D system is on the VBS side of a quantum phase transi-
tion. According to conventional finite-size scaling theory, 
the window around the critical point within which a sys-
tem of linear size $L$ exhibits scaling is proportional to 
$L^{-1/\nu}$, where $\nu$ is the exponent governing the divergence 
of the correlation length. Depending on the prefactor, 
this window may be sizable for practically reachable lat-
tice sizes. As will be shown next, this is one reason why 
fits to small-lattice data can give misleading results, e.g., 
in the case of $Q_2$-model results in Fig. 7.

In addition to illustrating the near-critical VBS, the 
scaling of the Néel order parameter will also be briefly 
discussed here. According to past studies, both the $J$-
$Q_2$ and $J$-$Q_3$ models are strong candidates for 
the deconfined quantum-criticality scenario, according 
to which both order parameters should be critical exactly 
at the same point. Results for the $J$-$Q_2$ model will be 
discussed here.

While all numerical results so far are consistent with a 
single Néel–VBS transition point, it has proved remark-
ably difficult to determine the location ($J/Q_2)_c$ of 
this transition precisely. The most recent QMC stud-
ies point to a continuous transition with unusually large 
scaling corrections in the quantities normally used to ex-
tract the critical point, e.g., the spin stiffness and Binder 
cumulants. These corrections have made it difficult 
to reliably extrapolate the critical coupling ratio ($J/Q_2)_c$ 
infinite size. By using a logarithmic scaling correction 
to the spin stiffness (which was not predicted in the 
original field-theory description of deconfined quantum-
critical points but may appear with a modified action), 
($J/Q_2)_c = 0.0447 \pm 0.0002$ was obtained in Ref. 42. 
Using a conventional correction $\propto L^{-\omega}$, with small $\omega$ and a 
large prefactor (which potentially could be a consequence
of the dangerously irrelevant operator responsible for the $Z_4$ symmetric VBS, gives a similar result.

In Fig. 13 the two order parameters are graphed versus the system size on log-log scales for coupling ratios close to the critical value. The Néel order parameter $\langle M^2 \rangle$ (the squared sublattice magnetization) is the size-normalized $(\pi, \pi)$ Fourier transform of the spin correlation function $\langle S_i S_j \rangle$. Both order parameters indeed exhibit critical scaling at $(J/Q_2) = 0.0447$. For other couplings the curves fan out in the way typical for critical points.

Interestingly, at $J/Q_2 = 0.0447$ both order parameters scale as $L^{-1+\eta}$ with $\eta \approx 0.27$ (with a purely statistical error bar of about 0.01) when $L \leq 32$ systems are used in the fits. For the sublattice magnetization, this exponent is slightly smaller than in previous works, while the VBS exponent is somewhat larger than in previous works, and if these exponents are truly exactly the same, it would imply a duality of the effective low-energy field theory that had not been anticipated, but further detailed work, using larger system sizes and studying several coupling ratios in the neighborhood of $J/Q_2 = 0.0447$, will be required before such a claim can be made and also be a coincidence that the two exponents are almost equal. Note also that the value of $\eta$ quoted here may also still be affected by sub-leading scaling corrections.

For coupling ratios larger than the critical value, in Fig. 13 exemplified by $J/Q_2 = 0.1$, the VBS order parameter turns downward, reflecting the faster decay to zero. Asymptotically, at the Néel state the decay should follow the $1/L^2$ form, but this can only be observed when the lattice size exceeds the correlation length (which is very large this close to the critical point). The sublattice magnetization turns upward, reflecting an extrapolation to a non-zero value. For smaller $J/Q_2$, here 0 and 0.03, the behavior is the opposite, reflecting a VBS state with no coexisting VBS order.

For the present purpose of detecting VBS order, an important aspect of the critical scaling is that, once a critical point has been identified, upward deviations from the power-law scaling, as seen in Fig. 13 at $J/Q_2$ = 0 and 0.03, still can demonstrate an ordered state when moving away from criticality. It may be easier, in many models, to establish a critical point (or a first-order transition) than to accurately extrapolate the infinite-size value of the order parameter in a state with significant fluctuations (an order parameter significantly smaller than its maximum possible value). Based on the knowledge of the existence of a phase transition, it may be possible to establish long-range order even in the presence of strong quantum fluctuations. This will be the case especially in calculations limited to much smaller systems.

IV. BOUNDARY SYMMETRY BREAKING

One interesting aspect of the results presented in the previous section, exemplified in Figs. 13 and 14 is that the boundary conditions dictate which of the order parameters, $\langle D_x^2 \rangle$ or $\langle D_y^2 \rangle$, is the one surviving in the thermodynamic limit. For 90° rotationally-symmetric periodic $L \times L$ lattices both order parameters are of course equal by symmetry (and spontaneous symmetry breaking in the thermodynamic limit will randomly select one of the directions), but in other cases only one of them should survive in the thermodynamic limit (i.e., the lattice shape acts like a symmetry-breaking field). Exactly how the symmetry is broken should be model dependent, and also dependent on fine details of the boundary conditions. Note that there are no “neutral” boundaries for a VBS, i.e., any boundary conditions should favor one component of the order parameter above the other (expect perhaps for some unusual fine-tuned boundaries with adjustable couplings).

Here the $Q_2$ and $Q_3$ models will be used to illustrate the complexity of the boundary issues further, with direct measurements of the order-parameter components $\langle D_x \rangle$ and $\langle D_y \rangle$ in systems where the edges break either the x-translational symmetry or both the $x$ and $y$ symmetries. The boundary effects are particularly interesting in view of the emergent U(1) symmetry, due to which both order parameter components can survive up to large system sizes, as already shown in Sec. III B in the case of periodic systems. Here the ability of boundaries to twist the local order parameter in the $(D_x, D_y)$ plane will be studied.

Two types of $2L \times L$ cylindrical lattices will be used. In addition to the case discussed so far, where the $y$-oriented edges are open and uniform, a modified boundary that breaks the translational symmetry in the $y$ direction will also be studied. The modification acts as a field inducing $D_y$ order at the edges. It is interesting to observe the interplay of this effect and the competing effect of the open boundary to lock in $D_x$ ordering when $L_x$ is even (as demonstrated in Fig. 6). This aspect of the VBS ordering is also important in view of DMRG studies, where modified boundaries are often used. Here the boundary modification will simply be accomplished by excluding from the Hamiltonian the $Q_2$ or $Q_3$ terms with vertical bonds closest to an edge on every second row, as illustrated in Fig. 14 in the case of $Q_2$ terms. Results obtained with only one of the edges modified will be compared with the case of both edges modified in the same way.

The local variations of the VBS vector order parameter $(D_x, D_y)$ of the $J-Q_2$ model were previously investigated...
for $L \times L$ lattices with all open edges. The formation of a vortex-like structure in the order parameter was noted. In the cases studied here, there is still translational symmetry with period two along the $y$-axis and, therefore, a 1D description of the order parameter as a function of the $x$ coordinate suffices. The local $x$ and $y$ order parameters are defined using the dimer operator $B_x$ in Eq. (11):

$$D_x(x) = \left[ \langle B_x(x, y) \rangle - \frac{1}{2} \langle B_x(x - 1, y) \rangle \right] \left( -1 \right)^x,$$

$$D_y(x) = \left[ \langle B_y(x, y) \rangle - \langle B_x(x, y + 1) \rangle \right] \left( -1 \right)^y. \quad (21)$$

These quantities are independent of the $y$ coordinate (and an average is taken in the simulations to improve the statistics). A VBS angle $\theta(x)$ can also be defined,

$$\theta(x) = \arctan \left( \frac{D_y(x) + D_y(x + 1)}{2D_x(x)} \right), \quad (22)$$

such that $\theta = 0$ and $\theta = \pi$ for a fully $x$ or $y$ oriented VBS order, respectively. The reason for using the sum $D_y(x) + D_y(x + 1)$ in the numerator under $\arctan()$ is that an $x$-oriented column of bonds labeled by $x$ is located between the $y$-oriented columns at $x$ and $x + 1$ (although such a detail of the definition of the local angle is not strictly important, and there are other equally good definitions giving the same result for large systems).

Fig. 15 shows results for the $Q_2$ model with only one modified edge. Oscillations in the bare dimer expectation value $\langle B_x(x) \rangle$ are present (top panel as in the case of the uniform edge in Fig. 6) In this case, however, the function is not reflection symmetric, due to the unequal left and right edges of the cylinder. The order parameter $D_x(x)$ is the largest at the edges. Away from the edge it decays toward a value at the center of the system which is somewhat smaller than the locked-in order parameter previously extracted based on the data in Fig. 4 (which can be seen by analyzing data for several system sizes, not shown here). This is because the modified edge also leads to some amount of $y$ order (middle panel of Fig. 15) and although this induced order decays rapidly when moving away from the modified edge it does not go away completely, even close to the opposite edge.

The rather smooth decay of the $y$ order to almost zero at the opposite edge can be explained as due to the open edge strongly favoring $x$ ordering in its vicinity, even with the modification that breaks the $y$ translational symmetry. The modified edge therefore induces both $x$ and $y$ order, i.e., the VBS angle (22) is $0 < \theta < \pi/2$. Since the second edge does not break the $y$ translational symmetry explicitly, the $x$ ordering can completely dominate there, leading to a very small $D_y$. The smooth transition from mixed $x$ and $y$ to almost pure $x$ order is seen clearly in the VBS angle graphed in the bottom panel of Fig. 15. Away from the edges, the total order parameter for large systems, $D = (\langle D_x \rangle^2 + \langle D_y \rangle^2)^{1/2}$, approaches the value extracted for this model in the previous section. A maximum in the angle develops with increasing size close to the modified edge.

Fig. 16 shows results for systems with the $y$ symmetry broken at both edges. Also in this case it would appear that both the $x$ and $y$ order parameters survive throughout the whole system in the thermodynamic limit. Convergence of both components as well as the angle at the center of the system is seen. The VBS angle here being only slightly less than $\pi/2$ corresponds to an almost equal mixture of $x$ and $y$ order.

In spite of the apparent convergence of the VBS angle to a value close to $\pi/2$ in Fig. 16, the survival of both $x$ and $y$ order in the thermodynamic limit due to the modified edge is illusory. Since the VBS order is columnar, eventually, for very large systems, one would expect only $x$ or only $y$ order to survive. The explanation of the behavior seen is again the very large $U(1)-Z_4$ crossover scale in the $Q_2$ model (as discussed in Appendix A). It is then interesting to look at the same quantities in the $Q_3$ model, where there is no clear $U(1)$ symmetry (as also shown in Appendix A), i.e., the length-scale $\Lambda$ is very short in this case. Results analogous to those in Fig. 10 for the $Q_2$ model are shown in Fig. 17 for the $Q_3$ model. In this case, one can see clearly how the
FIG. 16: (Color online) Location dependent expectation values of the $x$ and $y$ VBS order-parameter components, Eqs. (20) and (21), of the $Q_3$ model on $2L \times L$ cylinders with both edges modified by a symmetry-breaking perturbation (favoring $y$-oriented bond order). The corresponding VBS angle extracted using Eq. (22) is shown in the bottom panel. The horizontal dashed line is at $\Theta = \pi/4$ (corresponding to equal $x$ and $y$ order parameter parameters).

FIG. 17: (Color online) Same as Fig. 16 for the $Q_3$ model.

y component vanishes with increasing system size away from the edges, while the $x$ order stabilizes to a constant value. Since the $x$ component is the surviving one, its approach to its bulk value should be governed by the standard VBS correlation length $\xi$. The decay of the $y$-component should reflect $\Lambda$, however (since the presence of $y$ order is due to the angular twisting of the order parameter). This is a direct physical method to access the $\text{U}(1)$ length-scale, providing an attractive alternative to studying the order-parameter distributions discussed in Appendix A.

The decays of the two componentss are analyzed quantitatively for a larger system in Fig. 18. Excluding the points immediately adjacent to the edge, the decays are of almost pure exponential form (with an even-odd effect seen for the $y$ component), giving $\xi = 1.9$ extracted from the $x$ component and $\Lambda = 6.5$ from the $y$ component. A similar analysis for the $Q_2$ model (not shown here), based on systems with up to $128 \times 64$ sites, gives $\xi \approx 25$ (and $\Lambda$ much larger still), but this estimate is not reliable because the form of the decay is affected by the proximity to the critical point and is far from a pure exponential at the accessible distances. Larger system sizes are required in this case, especially for extracting $\Lambda$, which is larger than 100 lattice constants according to the analysis in Appendix A (perhaps being several hundred lattice constants). A systematic study of the divergence of the decay lengths of the $J$-$Q_3$ model upon approaching the quantum-critical point will be presented elsewhere.

FIG. 18: (Color online) The $x$ and $y$ components of the induced order parameter close to a modified edge of the $Q_3$ model on a $128 \times 64$ lattice. These data are the same as those shown in the top ($x$) and middle ($y$) panels of Fig. 16 for smaller systems, but with the non-zero constant behavior at the center of the system subtracted off in the case of the $x$ component. The lines are exponential fits, giving decay lengths 1.9 and 6.5 for the $x$ and $y$ components, respectively.
In the previous sections the 2D limit was approached in systems with fixed aspect ratio $L_x/L_y$. In principle the limit can also be accomplished with one of the lengths taken to infinity first, e.g., $L_x \to \infty$ for fixed $L_y$ and then $L_y \to \infty$. The behavior of the long-distance correlation functions, and, therefore, the squared VBS order parameter $Q$, should not necessarily be expected to be smooth, however. Although VBS ordering amounts to breaking a discrete symmetry, and order can therefore, in principle, exist for any $L_y$ in the infinitely long 1D cylinder geometry, the survival of the order for small $L_y$ is not guaranteed. Clearly, there will be enhanced fluctuations associated with the 1D nature of these systems, which may destroy the ground-state order of a Hamiltonian exhibiting long-range VBS order in the 2D limit.

A well known system with discrete symmetry breaking is useful for illustrating the potentially unsmooth 1D to 2D cross-over: The Ising model with nearest-neighbor coupling $J_z$ in a transverse magnetic field $h_x$ has a phase transition to an ordered (in the $z$ spin direction) state at a critical value $(h_x/J_z)_c$. On a 1D linear chain the critical ratio is $(h_x/J_z)_c = 1$, while on the 2D square lattice it is $(h_x/J_z)_c \approx 3.05$. For an $L_x \times L_y$ lattice with $L_x \to \infty$ one can expect $(h_x/J_z)_c$ to be a monotonic increasing function of $L_y$. Therefore, for a fixed

field $1 < h_x/J_z < 3.05$, one can expect cylinders with small $L_y$ to be disordered, while above some “critical” $L_y$ the system will be ordered. One can expect the same kind of behavior of a 2D VBS as well, when restricting it to a finite cylinder, unless the 2D order parameter is extremely large so that even the smallest cylinder remains in the ordered phase.

In the discussion below, only cylinders of even $L_y$ will be considered, so that the lattice is commensurate with columnar VBS order in both the $x$ and $y$ direction. $J$-$Q$ models with odd $L_y$ cannot be studied with the QMC method used here, because of sign problems arising due to geometric frustration of the spin interactions.

### V. LONG CYLINDERS

![FIG. 19: (Color online) VBS order parameter and correlations lengths on infinite ($L_x \to \infty$) $Q_2$ and $Q_3$ cylinders of width $L_y = 4, 6, 8, 10, 12$. (a) The correlation length extracted using the dimer correlations with $y$-oriented bonds as a function of $L_y$ for those cylinders that have disordered ground states (the $x$ correlation lengths are about $5 - 10\%$ smaller). (b) The order parameter versus $L_y$, along with the corresponding 2D order parameters (shown with the horizontal lines).](image1)

![FIG. 20: (Color online) VBS correlation functions, as defined in Eq. (20), for $y$-oriented dimers in the $Q_3$ model as a function of the separation in the $x$-direction on cylinders in the $L_x \to \infty$ limit. For $L_y = 4, 6$, fitted curves of the form $C \propto \exp(-x/\xi)/x^n$ to the $x \geq 4$ data are also shown (with $\alpha \approx 0.5$ in all cases).](image2)
dimer correlator, can be used to detect columnar VBS order with the bonds oriented either along the x or the y direction;

\[ S_{dx}(x) = \frac{1}{L_y} \sum_{y=0}^{L_y-1} [C_{dx}(x,y) - \frac{1}{2}C_{dx}(x-1,y) - \frac{1}{2}C_{dx}(x+1,y)], \]  
\[ S_{dy}(x) = \frac{1}{L_y} \sum_{y=0}^{L_y-1} C_{dy}(x,y)(-1)^y. \]  

(23)

(24)

Here it is appropriate to use periodic boundary conditions in both lattice directions. In order to achieve the limit \( L_x \to \infty \), aspect ratios \( L_x/L_y \) up to 32 were studied for \( L_y \) up to 12.

In the Q3 model, the y-dimer correlator \( S_{dy}(x) \) approaches a non-zero constant for large \( x \) when \( L_y \geq 8 \), as shown in Fig. 20, while for \( L_y = 4, 6 \) the correlations decays exponentially with distance. The behavior is not purely exponential but follow the form \( S_{dy}(x) \propto x^{-\alpha} \exp(-x/\xi) \), with \( \alpha \approx 0.5 \). This form with \( \alpha = 1/2 \) is the Ornstein-Zernike (mean-field) form expected in a \( d = (1 + 1) \) dimensional system, where \( \alpha = (d - 1)/2 \).

The correlation lengths extracted from fits to this form (with \( \alpha \) regarded as a free parameter, to produce somewhat better fits) are shown in Fig. 19(a). The x-oriented correlation function \( S_{dx}(x) \) is exponentially decaying for all \( L_y \), i.e., these systems are purely \( y \)-ordered in the thermodynamic limit (as was also found in Sec. III.B) for periodic \( 2L \times L \) systems when \( L \to \infty \). For \( L_y = 4, 6 \) the \( x \) correlation lengths are slightly smaller than the \( y \) ones. The \( y \) correlation lengths are graphed in Fig. 19(a).

In Fig. 22 both the \( x \) and \( y \) correlation functions for the Q2 model are graphed for all even-width cylinders with \( L_y = 4, \ldots, 12 \), along with fits to the exponential form discussed above. The \( y \) correlation length \( \xi_y \) is the larger one (about 5–10% larger than \( \xi_x \)) and is graphed versus \( L_y \) in Fig. 19(a). The correlation length grows roughly linearly with \( L_y \) for these cylinders. It would be interesting to go even larger \( L_y \) to study the form in greater detail, and of course to find the threshold width for ordering in this case (where presumably the correlation length should diverge, if one regards \( L_y \) as a continuous parameter). The rather small correlation lengths for \( L_y \) up to 12 suggest that it may be difficult to reach the critical width with QMC calculations at present.

The destruction of the VBS order even on rather wide cylinders is surprising. In the Q3 model, judging by the decay of the \( x \) component of the order parameter in Fig. 18, the 2D correlation length is approximately 2 lattice constants. The lower width \( L_y = 8 \) for ordering on infinitely long cylinders is therefore roughly four times the correlation length. Moreover, related to the short correlation length, the 2D order parameter is as large as 70% of the classical value. One might have expected such a system to be describable essentially in terms of classical (orthogonal, hard-core) dimers with quantum fluctuations of the nature present in quantum dimer models.

It has been expected that a VBS under these conditions should be ordered even on narrow cylinders. The results obtained here suggest that the non-orthogonality of the singlets (the true quantum dimers) has a dramatic effect on cylinders, in contrast to this effect actually enhancing the dimmer-dimer correlations relative to those in corresponding dimer models in critical 2D systems. The other hand, to the author’s knowledge, quantum dimer models that order in the 2D limit have actually not been extensively studied in long-cylinder geometry. Such studies would clearly be worthwhile, in light of the surprising results obtained here.

In the Q2 model the correlation length should be in the range 20–30 (with, as already discussed above, the large uncertainty being due to the fact that system sizes \( L \gg \xi \) are needed to determine \( \xi \) accurately), and one can, thus, expect, roughly, \( L_y \approx 100 \) to be needed before ordering sets in on the cylinders in this case.

One might speculate that the emergent U(1) symmetry could play some role in destroying the VBS order on the long cylinders. The local coarse-grained VBS order parameter \( (D_x, D_y) \) is an essentially isotropic 2D vector up to a large length scale \( \Lambda \sim \xi^{1+\alpha} \) with \( \alpha > 0 \) (with the best estimate so far being \( \alpha = 0.20 \pm 0.05 \)). If the order parameter were truly a vector with isotropic angular fluctuations, long-range order on the 1D \( L_x \to \infty \) cylinders would be strictly prohibited. The almost continuous or-
der parameter could then be argued to contribute to the loss of order. If so, one would expect a critical state to replace long-range order, however, of which there are no signs here—the VBS order decaying exponentially starting from short distances. There is no cross-over from a critical behavior, which might have been expected if almost U(1) symmetric angular VBS fluctuations were responsible for the destruction of long-range order. The role of emergent U(1) symmetry on cylinders is nevertheless interesting and should be studied more systematically in the future.

Regardless of the exact relationship between the 2D correlation length and the ordering threshold on cylinders, the very short correlation lengths found in the $Q_2$ model (ranging from about $\xi \approx 2$ for $L_y = 4$ to $\xi \approx 8$ for $L_y = 12$) show the dangers of using the long-cylinder geometry for drawing conclusions about the presence or absence of VBS order in the 2D limit. Order likely appears in the $Q_2$ model, and probably in most models for which the existence of VBS order is under debate, for $L_y$ far exceeding the maximum size that can currently be studied (especially if QMC methods cannot be used and DMRG would be the best choice of method).

The above conclusions regarding ordered and disordered cylinders reached based on correlation functions in long periodic $L_x \times L_y$ systems can also be confirmed by examining open-edge cylinders, in which a unique VBS can be locked in for even $L_x$ (as discussed in the case of $2L \times L$ cylinders in the preceding sections). Fig. 22 shows results for longer $Q_3$ cylinders in which the boundary perturbation inducing $y$ order was also applied at both edges (as in Fig. 14). For $L_y = 4$, both order parameter components decay quickly away from the edges, while for $L_y = 8$ the $y$ component stabilizes at the center of the system, at a value agreeing with that extracted on the basis of the correlation functions [shown in Fig. 19(a)]. Here, although the open edges favor $x$ order more than the perturbations favor $y$ order, the $y$ component eventually wins because that is the component favored just by having a finite $L_y$, and this effect scales with $L_x$. In contrast, for the $2L \times L$ cylinders with the same types of edges, it is the $x$ component that survives in the thermodynamic limit, as seen in Fig. 17.

VI. CONCLUSIONS AND DISCUSSION

A. General summary and conclusions

Several bench-mark results for the finite-size behavior of the VBS order parameter have been presented in this paper. The $J$-$Q$ and pure $Q$ models allowed investigations of both strongly and weakly ordered ground states. The main general conclusion (which should be valid for VBS states in many systems) drawn from these studies is that even when the VBS order is relatively strong on the infinite 2D lattice (e.g., $10 - 20\%$ of the maximum value attainable), results for small and moderate lattices (e.g., with up to hundreds of spins) can exhibit nearly critical behavior. The squared VBS order parameter then appears to extrapolate to zero in the thermodynamic limit. In the $J$-$Q$ model, this behavior can be traced to a rather large quantum-critical scaling regime around the critical value of $J/Q$, where the behavior follows closely that obtaining at a critical point.

The extrapolation to infinite size may at first sight seem easier when symmetry-breaking boundaries are used (as is often done in the context of DMRG studies), so that the order parameter can be computed directly (having a considerably larger value than its square when the VBS order is not very strong). However, a small order parameter ($10 - 20\%$ of the maximum value in the VBS systems considered here) is very difficult to extrapolate accurately in this way, partially because the symmetry is not completely broken on lattices of size that can be studied in practice. In particular, the emergent U(1) symmetry of the VBS order parameter implies that the component not locked by the boundaries can survive in the form of significant fluctuations up to very large system sizes, but this aspect of the ordering may be completely missed if one only examines the boundary-induced component of the order parameter. While this effect by itself would probably not lead to wrong conclusions regarding the presence or absence of VBS order, it is still important for explaining results that would otherwise seem inconsistent with each other (e.g., when comparing the total squared order parameter and a direct boundary in-
duced order parameter, as was done here in Sec. III C. The results presented here suggest that the best quantity for extrapolating the order parameter to infinite system size is the total (sum of the $x$ and $y$ components) long-distance correlation functions on $L \times L$ periodic lattices. Non-square lattices can lead to non-monotonic finite-size behavior.

Some of the small-system behaviors pointed out here are generically well known and not limited to VBS order. There are also many examples of finite-size scaling of results for small lattices leading to wrong conclusions of the nature of the ground state. For example, in Refs. 98 and 99 a spin liquid ground state was claimed to exist in a 2D system of weakly coupled $S = 1/2$ Heisenberg chains. When QMC results for larger systems became available, they showed a cross-over of the scaling and an asymptotic behavior in accord with a Néel state for any value of the inter-chain coupling.

The additional complications due to emergent U(1) symmetry of VBSs was developed in the case of deconfined quantum-critical points and has been confirmed in the case of U(1) symmetry of VBSs was developed in the context of staggered VBS states. For a VBS there is no “neutral” edge; any boundary affects the ordering pattern in its neighborhood. While in the bulk VBS, in the thermodynamic limit, only one of the components can survive in a columnar state, at edges they can both be present. Due to the large length-scale of the cross-over from the U(1) symmetric order parameter, both components can also survive in the interior of large systems. It would be interesting to study this phenomenon also in systems with a more complicated (larger unit cell) VBS order parameter.

It should be noted that, although the concept of emergent U(1) symmetry of VBSs was developed in the context of deconfined quantum-critical points and has been confirmed in the case of $J$-$Q$ models, this aspect of VBS order is most likely very general and manifested also in systems that are not very close to such critical points—in some extended parameter space—in 2D systems in which “angular” VBS fluctuations are possible once the correlation length is several lattice constants or larger. The U(1) related boundary effects should be absent in cases where the angular fluctuations are absent, e.g., in the case of staggered VBS states.

For the purpose of detecting VBS order, an important aspect of the critical scaling is that, once a critical point has been identified, upward deviations from the power-law behavior, as seen in Fig. 13 at $J/Q_2 = 0$ and 0.03 in the $J-Q_2$ model, demonstrate an ordered state although this may not be apparent when carrying out extrapolations of the order parameter in $1/L$ (as in Fig. 1). In general, in a model with some tunable parameter that can bring it into or out of a VBS state, it may be easier to detect a phase transition than to extract the exact value of the order parameter close to such a point. On the one hand, many frustrated systems may have VBS states that are always only weakly ordered and, hence, close to a quantum critical point (or weakly first-order transition) in some extended parameter space. Such systems should exhibit near-critical scaling on small lattices. On the other hand, if no critical scaling can be detected, and instead the order parameter correlation function decays exponentially fast with distance (or shows a tendency to decay faster than a power law), one can rather safely conclude that there is no VBS long-range order. Also with this approach, one can of course not expect to draw reliable conclusions unless the system sizes are sufficiently large (and how large that is depends on the model).

A striking behavior that may be particularly prominent in the case of VBS order was found here for lattices in the form of long cylinders, of size $L_x \times L_y$ with $L_x \to \infty$ and finite even $L_y$. In this geometry the order is unstable, and the system exhibits only short-range VBS correlations, until $L_y$ exceeds some threshold that can be very large (perhaps 3-4 times the VBS correlation length, according to results for the $Q_3$ model). Long cylinders are therefore not ideally suited for determining the nature of the 2D state in which VBS order is a possibility (systems with a small fixed $L_x/L_y$ normally being better). In particular, the method of positively confirming a $Z_2$ spin liquid by the absence of order on even-$L_y$ systems is not applicable in the “yes-no” sense proposed in Ref. 83. Instead, the finite-size behavior has to be tracked as in any other extrapolation method. The correlation length as a function of even $L_y$ should converge for a spin liquid and diverge for a VBS, as in Fig. 19 but it may not be easy in practice to determine which of these behaviors applies.

B. Comment on the possibility of a spin-liquid state in the $J_1$-$J_2$ Heisenberg model

One motivation for the present study was to provide guidance on detecting VBS order—or, alternatively, showing the absence of such order—in calculations for frustrated 2D models. The lattice sizes reachable for such systems with unbiased calculations, primarily using the DMRG method, are still very limited. Methods based on tensor-product states are beyond matrix-product states (which are closely related to the DMRG scheme), are still typically too much affected by various truncation errors and approximations to be considered completely unbiased. The following discussion will therefore be primarily aimed at DMRG calculations, although many of the issues would apply more generally.

The issues raised here have particular relevance in the context of a recent DMRG study of the $J_1$-$J_2$ Heisenberg model on the square lattice. Several different ways of analyzing VBS correlations were argued to consistently show the absence of VBS order and positively confirm the properties of a $Z_2$ spin liquid. However, many of the results presented can also be explained by a VBS state, at least in some part of the non-magnetic phase, according to the results obtained here. The key points supporting this view are summarized next.
In Fig. 3 of Ref. 6, second-order polynomial fits to the VBS order parameter for $2L \times L$ cylinders with $L \leq 10$ are shown. The fact that these fits extrapolate to negative values in the thermodynamic limit was taken as evidence for the absence of VBS order. However, this kind of behavior is also observed for the $Q_2$ model on small lattices, as seen in Figs. 7 and 9 of the present paper, even though the order parameter of this model is as large as 20% of the maximum possible value. If VBS order exists also in the non-magnetic phase of the $J_1$-$J_2$ Heisenberg model, one should not expect it to be very strong. Therefore, the finite-size behavior seen in Fig. 3 of Ref. 6 is at least qualitatively what would be expected even if the state is a VBS. It should be noted that the fact that the fitted functions extrapolate to negative values is in itself a clear sign of the chosen functional forms not being correct, as the squared order parameter cannot be negative. Thus, there must necessarily be a cross-over to a different form for larger systems—either to a pure 1/$L^2$ form, if there is no long-range order, or to an exponentially rapidly convergent form tending to a non-zero value. The results for small systems cannot distinguish between these different asymptotics.

The finite-size extrapolation issues may clearly also affect the determination of the transition point between the Néel antiferromagnet and the non-magnetic state at $g = J_2/J_1 \approx 0.4$ (while the transition point into the stripe antiferromagnet at $g = J_2/J_1 \approx 0.6$ is much easier to extract due to it being clearly first order). The transition point $g \approx 0.41$ was determined in Ref. 6 based on extrapolations of the Néel order parameter ($M^2$) using second-order polynomials, and these should be affected by similar problems as those pointed out here for the VBS scaling (and it is also well known that polynomials higher than second order have to be used to extrapolate Néel order correctly based on small systems, even in the strongly order Heisenberg model\(^{27,41}\)). The Néel order should therefore survive up to somewhat larger $g$ values. Thus, at $g = 1/2$, on which most of the analysis of the VBS scaling was focused in Ref. 6, the system may be rather close to the transition point. If VBS order exists in the nonmagnetic phase, it would therefore likely be very weak at this point. In Fig. 3(a) of Ref. 6, the maximal value of the order parameter ($D_0^x$), at $g$ just below 0.6, is close to the values for the $Q_2$ model in Fig. 9 of the present paper. Thus, if the $J_1$-$J_2$ model has VBS order, its peak value should be about 10–20% of that of a perfect columnar state. It would be better to analyze the VBS correlations closer to the maximal value, where the extrapolation problems are minimized.

As discussed in Sec. 11, in systems where there is a quantum phase transition into the state of interest, the best way to deduce the nature of that state may be to first carefully examine the phase transition. If there is critical scaling, deviations from the power-law form of the order parameter away from the critical point can be a good signal of long-range order. However, as seen in the scaling plot for the near-critical $J$-$Q_2$ model in Fig. 23, if the accessible system sizes are only up to $L \approx 10$, even a system in which the VBS order parameter is as large as 20% of the maximum value may in practice not be distinguishable from a critical system when analyzing the order parameter fluctuations. If the non-magnetic state of the $J_1$-$J_2$ Heisenberg model also has long range order, then one should expect a similar behavior.

Re-plotting the $g = 0.5$ and 0.56 data for the VBS $y$ component of Fig. 3(a) of Ref. 6 on a log-log scale, one can indeed observe behaviors close to power laws, as shown in Fig. 23(a). In the same graph data for the $J$-$Q_2$ model at $J = 0$ and $J_c = 0.0447$ are also graphed. In this case the $x$ component of the order parameter is shown, which, as seen in Fig. 9 in this system is larger than the $y$ component and is the one surviving in the thermodynamic limit. In the $J$-$J_2$ model it is instead the $x$ component that is somewhat larger. The comparison of the two models is complicated by the fact that the average induced $x$ order was subtracted in the definition used in Ref. 6. That induced order is very small, however, unlike what it is in the $Q_2$ model (which, may indicate that the VBS order, if it exists in
the $J_1$-$J_2$ model, is $y$-oriented on the cylindrical $2L \times L$ systems, as was also noted in Ref. [4].

For the open-edge $2L \times L$ cylinders used in Fig. 23(a), the $J$-$Q_2$ results do not exhibit quite as good scaling as in the case of the periodic $L \times L$ systems in Fig. 13, but for large systems the behavior is still consistent with an exponent $\eta \approx 0.3$. The $J_1$-$J_2$ results for $g = 0.5$ follow a different behavior, however, decaying as $L^{-\alpha}$ with $\alpha \approx 1.8$. This is quite close to $\alpha = 2$, which is expected deep inside a non-VBS phase. For $g = 0.56$ the data for the larger sizes deviate significantly upward from the $g = 0.5$ points and cannot be fitted very well to a power law. The slope on the log-log scale is $\approx -1.52$ for a line drawn through the $L = 8$ and 10 points, but the data for smaller systems fall above the fitted line, showing a flattening out with increasing size. The reduction of the rate of decay is opposite to the expectation for a spin liquid and an indication that the system is VBS ordered in the infinite-size limit.

The behavior at $g = 0.5$ is puzzling. Since the VBS order parameter here follows quite close to the form expected in a spin liquid, one may conclude that this is what it is, and the deviations from the $\sim 1/L^2$ form are due to remaining size effects (i.e., the system size is not yet much larger than the correlation length). A possibility suggested by the behavior observed in Fig. 23 is that the $J_1$-$J_2$ model has a spin liquid phase following the Néel phase above $g \approx 0.4$, followed in turn by a VBS at larger $g$ (since the $g = 0.56$ results seem more indicative of weak VBS order). Another possibility is that there is no spin liquid, but the Néel–VBS transition takes place at $g$ significantly larger than previously believed, so that $g = 0.5$ would actually still be inside the Néel phase. Looking at the raw data for the sublattice magnetization in Fig. 2(a) of Ref. [4], it appears that this possibility cannot be ruled out (considering again also the fact that the second-order polynomial fits used should lead to an under-estimation of the critical $g$ where the Néel order vanishes). The behavior of the triplet gap in Fig. 2(b) seems to go against this scenario, however, although the way the gap was extracted, by targeting higher states obtained while keeping the edges in the ground state, may lead to strong corrections to the gap scaling.

To investigate possible near-criticality in the Néel order parameter, the results from Fig. 2(a) of Ref. [4] for $(M^2)$ at $g = 0.5$ are re-plotted on a log-log scale in Fig. 23(b). Interestingly, the behavior follows closely a power law, with an exponent $\eta$ very similar to that of the $J$-$Q_2$ model. This could indicate that the transition out of the Néel state indeed takes place close to $g = 0.5$ and is in the same universality class as the $J$-$Q_2$ model. Note that, within the deconfined quantum criticality theory this kind of criticality of the magnetic order would not necessarily require that the VBS order emerges at this point as well, because the exponents associated with the Néel order parameter are not affected by the VBS (since the operator causing the VBS order is dangerously invariant). Clearly there is not sufficient data here to make any firm conclusions about this scenario of a Néel to spin liquid transition, possibly followed by a subsequent liquid to VBS transition at higher $g$, but the behavior is intriguing and deserves further tests.

An important aspect of the analysis of Ref. [4], cited as positive evidence for a $Z_2$ spin liquid, is the behavior of the order parameter on infinitely long cylinders. There is an even-odd effect that had previously been found in liquid states of quantum dimer models. For odd $L_y$ and even $L_x \to \infty$, an $x$-oriented order parameter $\propto \exp(-L_y/\xi_y)$ is induced because of geometric frustration effects. For even $L_y$ no order is observed at all, regardless of the type of VBS (horizontal or vertical columns) favored by the edges. Unfortunately, odd-$L_y$ $J$-$Q$ cylinders cannot be studied with the QMC method used here, because of sign problems. However, based on the results presented here for even $L_y$ it is already clear that this kind of test for a $Z_2$ spin liquid may not be that useful in practice, because VBS order does not exist on the infinitely long cylinders (for $L_y$ up to some critical width that can be expected to be inaccessible in practice for systems that are weakly to moderately ordered in the 2D limit). In Ref. [4] it was implicitly assumed that any system with 2D VBS order will exhibit such order also on long thin cylinders.

It is also interesting to note that the induced order parameter as a function of the distance from a modified edge of systems in the $L_x \to \infty$ limit is very similar in the $J_1$-$J_2$ and $J$-$Q_2$ models. Fig. 24 shows results for the pure $Q_2$ model on cylinders of width $4$–$10$ in which the edge has been modified to break the $y$ translational symmetry, as discussed in Sec. [3] and illustrated in Fig. 14. Here cylinders with aspect ratio $L_x/L_y = 16$ were used (which is large enough to accurately represent

![Graph showing VBS order parameter component induced by edges modified to break the $y$ translational symmetry](image)

FIG. 24: (Color online) VBS $y$ order parameter component induced by edges modified to break the $y$ translational symmetry (as explained in Fig. 14) in the $Q_2$ model. Here $r$ is defined as the distance from the second column of spins away from the edge, since the edge modification extends to this location. The lines show exponential fits, with decay lengths 1.8 ($L_y = 4$), 3.2 ($L_y = 6$), 4.8 ($L_y = 8$), and 6.6 ($L_y = 10$).
the $L_x \to \infty$ limit). The edge-induced $x$ and $y$ order parameters both decay exponentially, with very similar decay lengths that are also close to the correlation lengths graphed in Fig. 12 (obtained from correlation functions on systems with all periodic boundaries). The $y$ decay lengths are always marginally larger. For $L = 6$ and 8, the decay lengths are about 1.5 times those in the $J_1$-$J_2$ model at $g = 0.5$, for which data were shown in Fig S6(b) of Ref. 4.

As discussed above and seen clearly in Fig. 23, the VBS order parameter is likely significantly suppressed at $g = 0.5$ relative to what it is close to its maximum in this model (which appears to be a bit above 0.56). One can therefore expect to see decay lengths as large as those in the $Q_2$ model for larger $g$ (close to 0.6). The rapid decay was in Ref. 4 interpreted as the system being insusceptible to VBS ordering even in the presence of, at first sight, very favorable conditions for inducing it. Again, when analyzed in light of the known physics of the $J$-$Q_2$ model, the results cannot be distinguished from those of a rather substantially ordered VBS. It would be illuminating to have $J_1$-$J_2$ data for $L_y > 8$, to see if the decay length continues to grow or saturates.

In Ref. 4 the size dependence of the entanglement entropy was also used as positive evidence of a $Z_2$ spin liquid. It would be very interesting to compute this quantity also for the $J$-$Q$ models. It is clear that the non-trivial aspects of the VBS fluctuations could lead to behaviors not predicted in the strong-VBS limit. Since the system on small lattices and cylinders resembles a spin liquid, it would not be surprising if the corrections to the area law of the entanglement entropy are also similar, up to some large size where the true asymptotic VBS behavior sets in. QMC calculations of the entanglement entropy of the $J$-$Q$ models will be carried out in future studies, using the recent developments of methods to study the Renyi versions of the entropies. This should clarify whether the constant deviation from the area law cited in Ref. 4 is really unique to $Z_2$ spin liquids, or whether they can also appear (for lattices of practically reachable size) in weakly ordered VBS states. The scaling of the entanglement entropy at a deconfined quantum-critical point is also of interest here.

The conclusion reached from the above comparisons of results for the $J_1$-$J_2$ model and the $J$-$Q$ models is that they exhibit rather similar behaviors, and, therefore, a VBS ground state of the $J_1$-$J_2$ cannot be excluded. Some of the $J_1$-$J_2$ results may also be consistent with a $Z_2$ spin liquid at $g \approx 0.5$, but the point to note here is that most of the results presented so far do not favor that kind of state over a VBS state. In particular, the claimed positive signals for a $Z_2$ spin liquid are also seen in the confirmed VBS state of the $J$-$Q$ models. If anything, the very similar behaviors seen in the near-critical $Q_2$ model and the $J_1$-$J_2$ models should tilt the balance further in favor of VBS order for $g = J_2/J_1$ close to 0.6. The behavior at $g = 0.5$ is very intriguing and not consistent with a near-critical VBS of the same kind as in the $J$-$Q$ models. It would be very useful to analyze the VBS and magnetic correlations further in this case, preferably on larger lattices.

It would also be good to know in greater detail the effects of truncation (the number of states kept) in the DMRG calculations. The error $\approx 10^{-7}$ in Ref. 6 refers to the missing weight in the density matrix. One can expect the errors in the wave function to be approximately the square-root of this error, but exactly how much the VBS correlations are affected, especially for the largest systems, is not entirely clear.

C. Remarks on other potential spin liquids

The results presented here also are relevant to studies of the kagome Heisenberg model, for which DMRG studies also have indicated a spin liquid state. A VBS is another candidate state which is not easy to exclude if the ordering is weak (which should be expected, if this kind of order is present). Since the most likely VBS patterns in this case are much more complicated than the columnar state of the $J$-$Q$ models discussed here (with the most likely candidate states having 12- or 36-spin unit cells), it is not possible to relate results in the same close manner as done above in the case of the $J_1$-$J_2$ model. Nevertheless, the issues pointed out here should be considered also when analysing the kagome system, in particular on long cylinders. It would be very desirable to reach larger $L_x \times L_y$ lattices with the aspect ratio $L_x/L_y$ kept fixed, although this seems difficult at present. It would also be good to push calculations based on the multi-scale entanglement renormalization ansatz (MERA) to higher precision. Such a calculation had previously seemed to confirm the VBS with 36-site cell proposed earlier based on other techniques, but the energy reached was not as low as that found with DMRG and exact diagonalization.

The analysis and arguments presented in this paper also suggest that it would be very useful to add to the nearest-neighbor Heisenberg exchange some term that favors one of the VBS states proposed previously, and to study the phase transition out of this ordered state. Longer-range couplings may work, but some interaction similar to the multi-spin $Q$ terms discussed here could be even better suited for inducing the desired type of VBS.

Spin liquid states have recently also been claimed to exist in electronic Hubbard models and frustrated spin models on the honeycomb lattice. The Hubbard model, 2D lattices with up to hundreds of sites were used. The VBS correlations in this case decay very rapidly with distance, and the system does not seem to exhibit the kind of problematic scaling issues pointed out in this paper. On the other hand, work on effective spin models constructed to capture the Putative spin liquid states have not so far been conclusive. It would be useful to extend the models in such a way that a VBS phase transition can be studied. The VBS
model combining the recently done in an exact diagonalization study of a 2D behavior when frustration is added to this model, as was it may be very useful to systematically investigate the quantum phase transitions. If the outcome is positive, these methods to capture non-trivial ground states and variations would be a very good test of the capabilities of behavior extracted on the basis of unbiased QMC simulations and support from Grant No. NTU 10R80909-4.

should then be the one to which the “bare” honeycomb model is the most susceptible (which may in itself not be easy to determine in this case).

D. Bench-mark challenge

Finally, as a challenge to DMRG, tensor-product, and MERA techniques, it would be very interesting and useful to see these methods applied to J-Q models as well. Comparing with the known phase diagram and critical behavior extracted on the basis of unbiased QMC simulations would be a very good test of the capabilities of these methods to capture non-trivial ground states and quantum phase transitions. If the outcome is positive, it may be very useful to systematically investigate the behavior when frustration is added to this model, as was recently done in an exact diagonalization study of a 2D model combining the Q2 interaction with the frustrated J1–J2 Heisenberg model.

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Appendix A: U(1)–Z4 cross-over of the VBS symmetry in periodic systems

The emergent U(1) symmetry of a columnar VBS in the neighborhood of a critical point can be characterized by the probability distribution \( P(D_x, D_y) \) generated in QMC simulations on periodic \( L \times L \) lattices. A systematic study aimed at extracting the scaling of the U(1)-Z4 cross-over length \( \Lambda \) was presented in Ref. Here additional results for the pure \( Q_2 \) and \( Q_3 \) models will be presented in order to facilitate comparisons with the boundary effects discussed in the main text. Specifically, it will be shown that the lack of \( D_x-D_y \) symmetry on \( 2L \times L \) lattices, as seen in Fig. for the \( Q_3 \) model for all system sizes, is matched by a clear \( Z_4 \) symmetric order parameter on all \( L \times L \) lattices. Conversely, the symmetry seen for the \( Q_2 \) model on large lattices in Fig. is consistent with only very small deviations (barely detectable) from U(1) symmetry on \( L \times L \) lattices with \( L \) as large as 128.

In the projector QMC simulations, each generated configuration is associated with a pair of order parameters \((D_x, D_y)\), which are matrix elements of the corresponding operators defined in Eqs. \( \text{(A1)} \) and \( \text{(A3)} \) computed in the valence bond basis. These matrix elements are of the form \( 3n/4N \), where \( n \) is an integer in the range \([-N/2, N/2]\), with the extremal values corresponding to both the bra and ket state (making up the transition graph) having the same perfect columnar pattern of valence bonds of length one lattice constant. The histogram \( P(D_x, D_y) \) is constructed based on these matrix elements.

Fig. 25 shows results for the \( Q_3 \) model for \( L = 12 \) and \( L = 24 \). In this model the histogram \( P(D_x, D_y) \) exhibits a distinct four-fold symmetry even for the smallest systems (also smaller than \( L = 12 \), not shown here, where the discreteness of the distribution function also becomes apparent). The four peaks sharpen with increasing lattice size, and above some size the suppression of the

![FIG. 25: (Color online) VBS order parameter distribution](image)

![FIG. 26: (Color online) Size dependence of the columnar anisotropy weight, defined in Eq. \( \text{(A1)} \), of the VBS order parameter distribution in the \( Q_3 \) model.](image)
weight between the peaks severely impedes QMC fluctuations between the peaks. In Fig. 25 the visibly different weight in the four peaks (with the right peak having the smallest weight) is a consequence of this rarity of “instanton” events between the peaks (i.e., the simulations “get stuck” in one quarter of the configuration space). It should be noted that this very slow simulation dynamics of the VBS order parameter does not affect the estimate of the total squared order parameter \( \langle D^2 \rangle \) and most other physical quantities of interest.

The degree of \( \mathbb{Z}_4 \) symmetry of the order parameter can be quantified by the function

\[
W_4 = \sum_{D_x} \sum_{D_y} P(D_x, D_y) \cos(4\phi_{xy}),
\]

where \( \phi_{xy} \) is the angle corresponding to the point \((D_x, D_y)\). While this function (and the underlying probability distribution) is not a physical observable, in the sense that it is not a bona fide quantum mechanical expectation value, it nevertheless reflects the fluctuations of the VBS order parameter and can be used to characterize the the U(1)-\( \mathbb{Z}_4 \) cross-over.

Results as a function of \( L \) for the \( \mathbb{Q}_3 \) model are shown in Fig. 26. Here the convergence \( W_4 \to 1 \) when \( L \to \infty \) is apparent, as would be expected for a columnar VBS in the thermodynamic limit. In principle the curve \( W_4(L) \) could be used to define the length \( \Lambda \), e.g., using \( W_4(\Lambda) = 1/2 \), but there is clearly an arbitrariness in choosing the particular number. For studying the scaling of \( \Lambda \) when some parameter of the Hamiltonian is changed (e.g., \( J/Q_3 \)) this ambiguity does not matter. In Ref. [41] curves \( W_4(L) \) for different coupling ratios were analyzed using standard finite-size scaling techniques, with the results that \( \Lambda \) grows slightly faster than the correlation length; \( \Lambda \sim \xi^{1+\alpha} \) with \( \alpha \approx 0.2 \).

Comparing with the behavior of the squared order parameters in Fig. 11 it can be noted that \( \langle D_x^2 \rangle \) approaches 0 (and \( \langle D_y^2 \rangle \) tends to a non-zero value) very quickly above \( L \approx 20 \), which is approximately where \( W_4(L) = 1/2 \) in Fig. 26. On the other hand, the decay of the edge-induced y component of the order parameter in Figs. 17 and 18 (where the system far from the edge has only x order) gives a length \( \approx 6.5 \), which could also be taken as a practical definition of \( \Lambda \). This length corresponds to \( W_4 \approx 0.1 \) in Fig. 26.

In contrast to the \( \mathbb{Q}_3 \) model, in the \( \mathbb{Q}_2 \) model no clear \( \mathbb{Z}_4 \) symmetry is visible in \( P(D_x, D_y) \) up to systems as large as \( L = 64 \) and 128, as shown in Fig. 27. These histograms are ring-shaped, although for \( L = 128 \) the weight is not evenly distributed because of lack of sufficient QMC statistics. The VBS angle fluctuates very slowly in simulations of large systems and very long runs are required in order to obtain symmetric distributions. The data shown are based on \( \approx 3.5 \times 10^8 \) Monte Carlo sweeps for \( L = 64 \) and \( 8 \times 10^7 \) for \( L = 128 \) (which required more than \( 10^4 \) CPU hours in both cases). By symmetrizing the distributions using \( 90^\circ \) rotations, one can still detect small deviations from perfect U(1) symmetry, as shown in Fig. 28. The peak positions again correspond to a columnar state.

Note that in Fig. 27 the ring for \( L = 128 \) is considerably thinner than for \( L = 64 \), with the radius (the location of the maximum or average weight) remaining almost unchanged. This reflects an expected reduction of the fluctuations of the magnitude of the VBS order parameter with increasing system size.

Based on these results, the cross-over length-scale \( \Lambda \) for the \( \mathbb{Q}_2 \) model should be \( \gg 128 \), which explains why both order-parameter components are essentially equal for the largest systems in Fig. 8.
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